



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:16 PM EDT

PDB ID : 7BYQ / pdb_00007byq
Title : The mutant variant of PNGM-1. H279A was substituted for alanine to study metal coordination.
Authors : Park, Y.S.; Kang, L.W.; Lee, J.H.
Deposited on : 2020-04-24
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

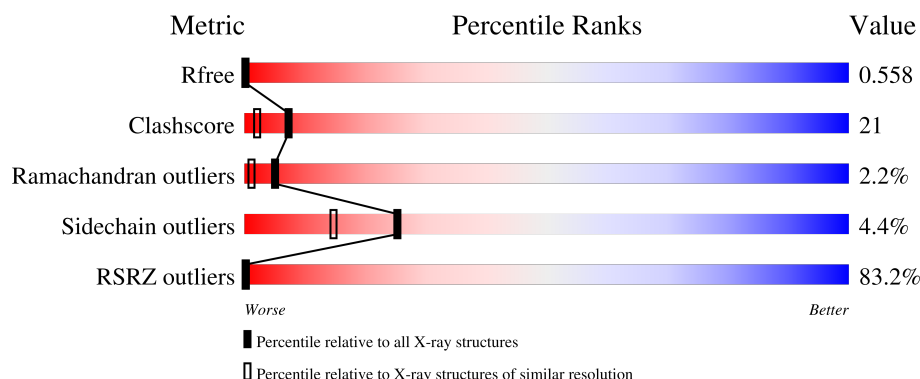
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	69% 64% 31%
1	B	372	80% 64% 30%
1	C	372	92% 61% 34%
1	D	372	83% 69% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11914 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Metallo-beta-lactamase PNGM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2851	1805	490	536	20			
1	B	360	Total	C	N	O	S	0	0	0
			2823	1789	481	533	20			
1	C	360	Total	C	N	O	S	0	0	0
			2823	1789	481	533	20			
1	D	362	Total	C	N	O	S	0	0	0
			2847	1804	487	536	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
B	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
C	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
D	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

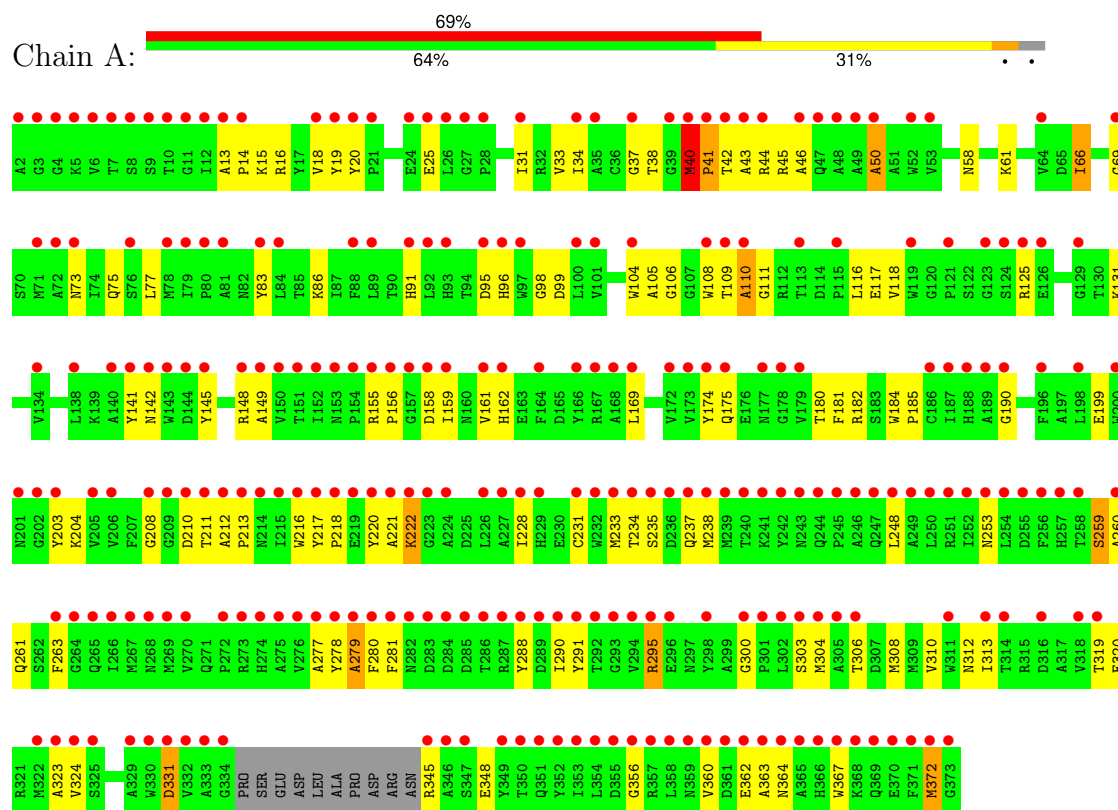
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	144	Total 144	O 144	0	0
3	C	148	Total 148	O 148	0	0
3	D	129	Total 129	O 129	0	0

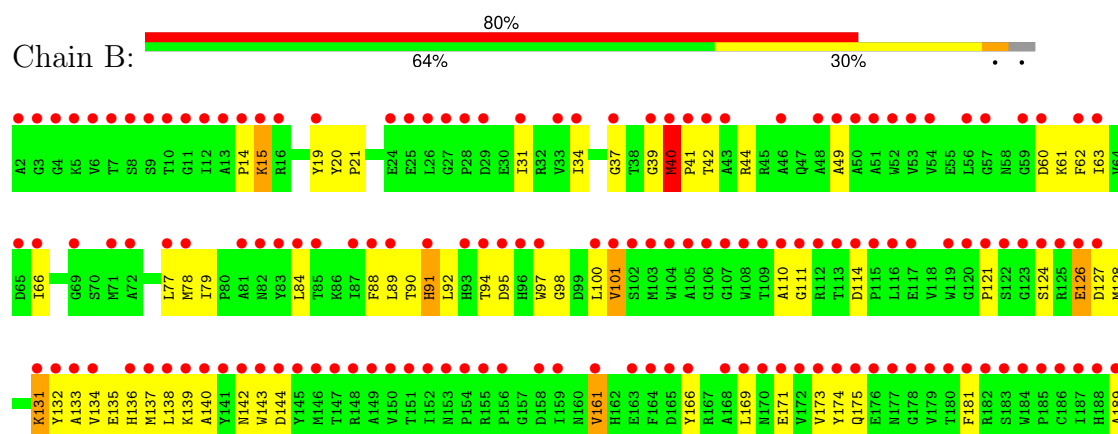
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Metallo-beta-lactamase PNGM-1

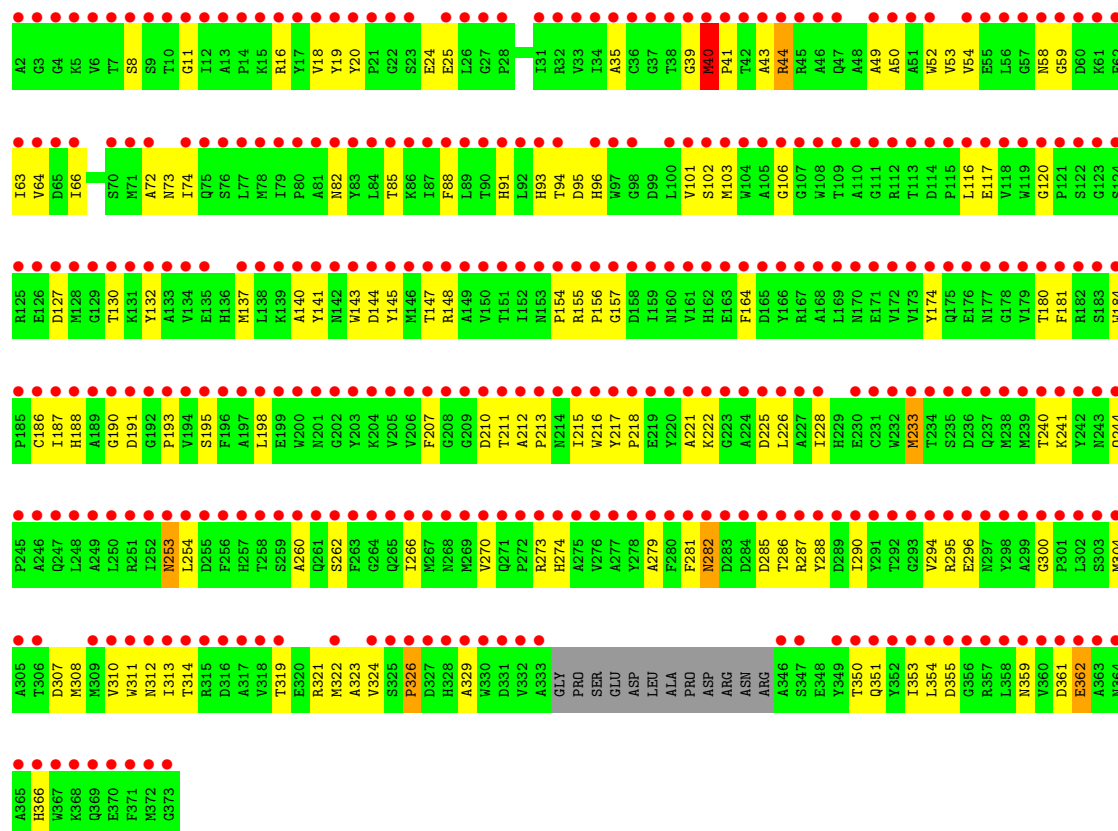


• Molecule 1: Metallo-beta-lactamase PNGM-1

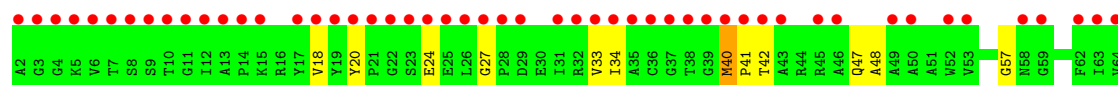
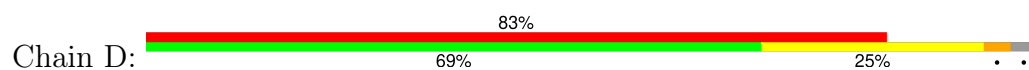


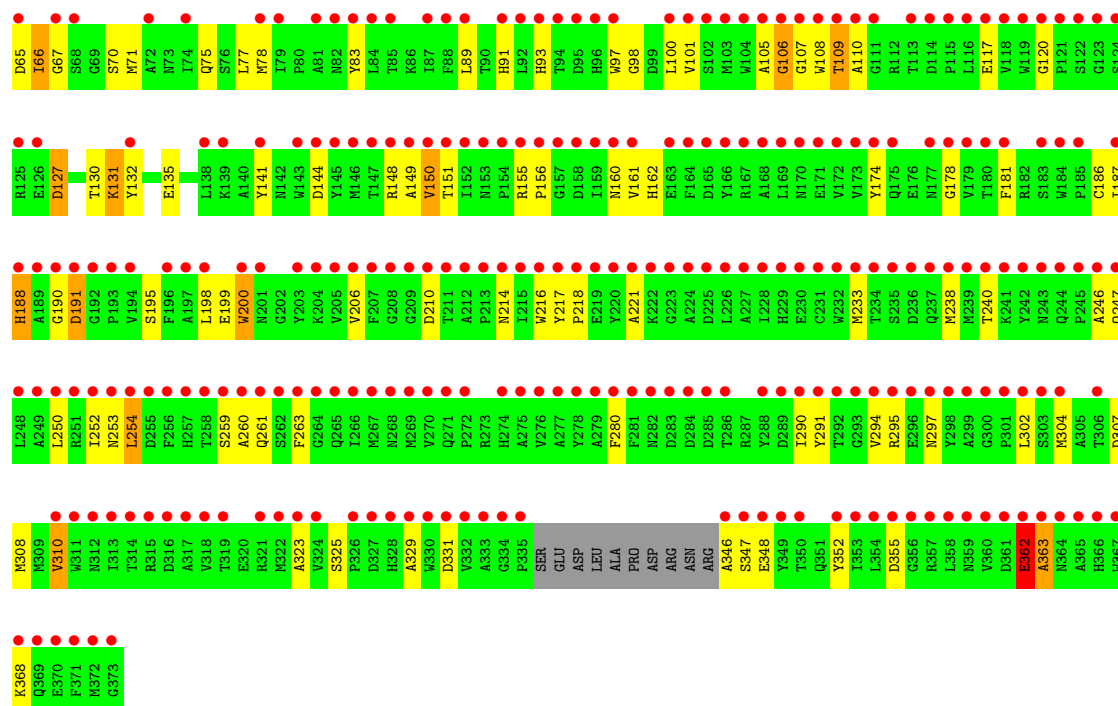


• Molecule 1: Metallo-beta-lactamase PNGM-1



• Molecule 1: Metallo-beta-lactamase PNGM-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.38Å 83.06Å 163.58Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	49.04 – 1.96 49.04 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.04-1.96) 97.2 (49.04-1.96)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.519 , 0.557 0.520 , 0.558	Depositor DCC
R_{free} test set	10778 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	11914	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0365e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	0/2933	1.42	5/3995 (0.1%)
1	B	1.08	0/2905	1.46	7/3960 (0.2%)
1	C	1.05	0/2905	1.42	1/3960 (0.0%)
1	D	1.05	0/2930	1.46	6/3993 (0.2%)
All	All	1.06	0/11673	1.44	19/15908 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	GLU	CB-CG-CD	6.83	124.20	112.60
1	D	346	ALA	CA-C-N	6.39	130.40	120.75
1	D	346	ALA	C-N-CA	6.39	130.40	120.75
1	D	263	PHE	CA-C-N	5.94	126.57	119.98
1	D	263	PHE	C-N-CA	5.94	126.57	119.98
1	D	127	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	190	GLY	CA-C-O	-5.61	116.24	121.96
1	D	346	ALA	O-C-N	5.46	131.73	123.00
1	B	131	LYS	N-CA-C	-5.31	105.38	111.07
1	B	193	PRO	N-CA-C	5.29	119.88	111.26
1	B	95	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	259	SER	CA-C-N	5.27	127.35	120.28
1	A	259	SER	C-N-CA	5.27	127.35	120.28
1	A	125	ARG	CA-C-N	5.08	127.40	120.54
1	A	125	ARG	C-N-CA	5.08	127.40	120.54
1	C	326	PRO	CB-CA-C	-5.08	105.10	111.71
1	B	131	LYS	CB-CG-CD	5.03	122.86	111.30
1	B	131	LYS	CA-C-N	5.01	127.00	120.28
1	B	131	LYS	C-N-CA	5.01	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2851	0	2683	113	0
1	B	2823	0	2641	124	0
1	C	2823	0	2641	137	0
1	D	2847	0	2677	102	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	145	0	0	46	0
3	B	144	0	0	64	0
3	C	148	0	0	69	0
3	D	129	0	0	54	0
All	All	11914	0	10642	452	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (452) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:MET:HE3	3:C:599:HOH:O	1.32	1.29
1:C:187:ILE:HB	3:C:568:HOH:O	1.37	1.20
1:B:213:PRO:HA	3:B:574:HOH:O	1.39	1.18
1:D:210:ASP:OD2	3:D:501:HOH:O	1.62	1.15
1:B:310:VAL:HB	3:B:593:HOH:O	1.49	1.12
1:C:210:ASP:OD2	3:C:501:HOH:O	1.65	1.11
1:D:233:MET:SD	3:D:599:HOH:O	2.07	1.10
1:A:204:LYS:NZ	1:A:220:TYR:O	1.88	1.04
1:C:266:ILE:HG21	3:C:583:HOH:O	1.60	1.01
1:D:40:MET:HB3	1:D:41:PRO:HD2	1.44	0.98
1:C:188:HIS:CD2	3:C:600:HOH:O	2.15	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ALA:HA	3:A:575:HOH:O	1.62	0.97
1:A:312:ASN:HB2	3:A:605:HOH:O	1.64	0.95
1:C:294:VAL:HG23	3:C:532:HOH:O	1.67	0.94
1:A:184:TRP:CZ2	3:A:608:HOH:O	2.20	0.94
1:B:124:SER:CB	3:B:506:HOH:O	2.16	0.94
1:D:214:ASN:HB3	3:D:588:HOH:O	1.69	0.91
1:B:132:TYR:CD2	3:B:559:HOH:O	2.23	0.91
1:A:105:ALA:HB1	3:D:554:HOH:O	1.71	0.90
1:B:40:MET:HB2	1:B:41:PRO:CD	2.02	0.90
1:B:166:TYR:CZ	3:B:573:HOH:O	2.24	0.89
1:D:40:MET:HB3	1:D:41:PRO:CD	2.04	0.88
1:A:108:TRP:HH2	3:A:504:HOH:O	1.56	0.88
1:B:37:GLY:HA3	1:B:49:ALA:O	1.74	0.88
1:B:126:GLU:O	3:B:501:HOH:O	1.92	0.87
1:A:25:GLU:OE2	3:A:501:HOH:O	1.91	0.87
1:A:217:TYR:CD2	3:A:608:HOH:O	2.27	0.86
1:C:311:TRP:CD1	3:C:587:HOH:O	2.29	0.85
1:A:149:ALA:HB2	3:A:504:HOH:O	1.75	0.85
1:B:286:THR:HG22	3:B:632:HOH:O	1.76	0.84
1:A:210:ASP:OD2	3:A:502:HOH:O	1.96	0.84
1:C:88:PHE:CZ	3:C:610:HOH:O	2.31	0.84
1:D:75:GLN:HB2	3:D:514:HOH:O	1.77	0.84
1:B:79:ILE:O	3:B:502:HOH:O	1.96	0.83
1:B:97:TRP:HB2	3:B:575:HOH:O	1.77	0.82
1:D:89:LEU:HD22	3:D:568:HOH:O	1.78	0.82
1:C:312:ASN:OD1	3:C:502:HOH:O	1.96	0.82
1:B:173:VAL:HG23	3:B:614:HOH:O	1.79	0.81
1:C:266:ILE:HD13	3:C:583:HOH:O	1.79	0.80
1:A:46:ALA:HB3	3:A:543:HOH:O	1.82	0.80
1:B:124:SER:HB3	3:B:506:HOH:O	1.78	0.80
1:B:286:THR:CG2	3:B:632:HOH:O	2.29	0.80
1:C:221:ALA:HB2	3:C:608:HOH:O	1.82	0.80
1:A:184:TRP:HZ2	3:A:608:HOH:O	1.60	0.79
1:A:313:ILE:HG22	3:A:552:HOH:O	1.83	0.79
1:C:191:ASP:O	3:C:503:HOH:O	2.01	0.79
1:C:143:TRP:CD1	3:C:599:HOH:O	2.35	0.77
1:B:134:VAL:HG23	3:B:533:HOH:O	1.85	0.77
1:B:40:MET:HB2	1:B:41:PRO:HD2	1.64	0.77
1:A:161:VAL:HG13	3:A:554:HOH:O	1.84	0.77
1:A:83:TYR:CD2	3:B:634:HOH:O	2.38	0.76
1:C:260:ALA:HB1	3:C:532:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PRO:HB3	3:C:613:HOH:O	1.84	0.76
1:A:40:MET:HB3	1:A:41:PRO:HD2	1.65	0.76
1:A:203:TYR:CE1	3:A:552:HOH:O	2.39	0.76
1:A:319:THR:HB	3:A:605:HOH:O	1.85	0.76
1:A:217:TYR:CE2	3:A:608:HOH:O	2.39	0.75
1:B:171:GLU:OE1	3:B:503:HOH:O	2.04	0.75
1:A:203:TYR:CZ	3:A:552:HOH:O	2.40	0.75
1:C:74:ILE:O	3:C:504:HOH:O	2.04	0.74
1:D:260:ALA:HA	3:D:569:HOH:O	1.87	0.74
1:D:294:VAL:CG2	3:D:569:HOH:O	2.35	0.74
3:B:506:HOH:O	1:C:350:THR:HG23	1.87	0.74
1:D:294:VAL:HG22	3:D:569:HOH:O	1.88	0.73
1:A:261:GLN:OE1	1:A:261:GLN:N	2.21	0.73
1:B:94:THR:HG22	1:C:141:TYR:CD1	2.24	0.73
1:C:72:ALA:O	3:C:505:HOH:O	2.06	0.73
3:B:522:HOH:O	1:C:353:ILE:HG12	1.88	0.73
1:A:253:ASN:ND2	3:A:506:HOH:O	2.22	0.72
1:A:364:ASN:ND2	3:A:505:HOH:O	2.22	0.72
1:A:118:VAL:HB	3:A:554:HOH:O	1.89	0.71
1:D:355:ASP:HB3	3:D:531:HOH:O	1.87	0.71
1:D:97:TRP:HB3	3:D:568:HOH:O	1.90	0.71
1:C:94:THR:HB	3:C:566:HOH:O	1.90	0.71
1:B:126:GLU:HG2	3:B:559:HOH:O	1.89	0.71
1:B:60:ASP:CB	3:B:540:HOH:O	2.37	0.71
1:B:268:ASN:O	1:B:271:GLN:HG2	1.92	0.70
1:B:346:ALA:O	3:B:504:HOH:O	2.10	0.69
1:C:212:ALA:HB3	3:C:568:HOH:O	1.93	0.69
1:D:290:ILE:HD13	3:D:544:HOH:O	1.93	0.69
1:C:174:TYR:CD1	3:C:610:HOH:O	2.46	0.68
1:B:194:VAL:HG13	3:B:513:HOH:O	1.92	0.68
1:A:98:GLY:O	3:A:503:HOH:O	2.12	0.68
1:B:193:PRO:HD2	3:B:511:HOH:O	1.93	0.68
1:A:61:LYS:O	1:A:86:LYS:NZ	2.27	0.68
1:B:191:ASP:HB3	3:B:573:HOH:O	1.93	0.68
1:B:144:ASP:OD2	1:C:94:THR:HG23	1.94	0.67
1:C:143:TRP:HD1	3:C:599:HOH:O	1.74	0.67
1:D:71:MET:HG3	3:D:514:HOH:O	1.94	0.67
1:B:210:ASP:OD2	3:B:505:HOH:O	2.11	0.67
1:D:186:CYS:SG	1:D:195:SER:OG	2.52	0.67
1:A:40:MET:HB3	1:A:41:PRO:CD	2.24	0.67
1:C:43:ALA:HA	3:C:545:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TYR:HD2	3:B:559:HOH:O	1.71	0.66
1:C:294:VAL:CG2	3:C:532:HOH:O	2.35	0.66
1:A:20:TYR:CD2	1:B:20:TYR:HB3	2.30	0.66
1:B:261:GLN:N	1:B:261:GLN:OE1	2.29	0.65
1:C:52:TRP:O	3:C:506:HOH:O	2.14	0.65
1:D:187:ILE:HD12	3:D:588:HOH:O	1.96	0.65
1:C:53:VAL:HG22	3:C:506:HOH:O	1.97	0.65
1:A:96:HIS:NE2	3:A:502:HOH:O	2.29	0.65
1:B:225:ASP:O	1:B:273:ARG:HB2	1.97	0.64
1:B:19:TYR:CB	1:B:310:VAL:HG11	2.27	0.64
1:C:40:MET:HE1	1:C:50:ALA:HB2	1.78	0.64
1:D:233:MET:HE1	3:D:575:HOH:O	1.96	0.64
1:B:191:ASP:OD2	3:B:506:HOH:O	2.14	0.64
1:C:66:ILE:N	1:C:96:HIS:O	2.29	0.64
1:C:103:MET:SD	3:C:558:HOH:O	2.55	0.64
1:C:188:HIS:HD2	3:C:600:HOH:O	1.64	0.63
1:A:182:ARG:HD2	3:A:629:HOH:O	1.99	0.63
1:B:282:ASN:HD22	1:B:306:THR:HB	1.63	0.63
1:A:238:MET:HG3	3:A:506:HOH:O	1.98	0.63
1:C:40:MET:SD	1:C:279:ALA:HA	2.39	0.63
1:D:260:ALA:CA	3:D:569:HOH:O	2.43	0.62
1:D:260:ALA:HB1	3:D:569:HOH:O	1.99	0.62
1:C:120:GLY:C	3:C:509:HOH:O	2.41	0.62
3:B:519:HOH:O	1:C:215:ILE:HG21	1.98	0.62
1:C:49:ALA:HB1	1:C:95:ASP:HB2	1.82	0.61
1:A:58:ASN:HA	3:A:621:HOH:O	2.00	0.61
1:C:262:SER:HB3	3:C:627:HOH:O	1.98	0.61
1:D:261:GLN:N	1:D:261:GLN:OE1	2.33	0.61
1:C:39:GLY:C	1:C:40:MET:SD	2.84	0.61
1:B:92:LEU:HA	1:B:97:TRP:CD1	2.34	0.61
1:B:40:MET:CB	1:B:41:PRO:CD	2.79	0.61
1:D:290:ILE:CD1	3:D:544:HOH:O	2.48	0.61
1:D:260:ALA:CB	3:D:569:HOH:O	2.47	0.61
1:A:363:ALA:HB3	3:A:505:HOH:O	2.00	0.61
1:A:98:GLY:C	3:A:503:HOH:O	2.43	0.60
1:C:24:GLU:OE1	3:C:507:HOH:O	2.16	0.60
1:A:18:VAL:HG23	3:A:596:HOH:O	2.02	0.60
1:C:295:ARG:HG2	3:C:531:HOH:O	2.01	0.60
1:D:105:ALA:O	1:D:148:ARG:NH1	2.29	0.60
1:C:130:THR:HB	3:C:509:HOH:O	2.00	0.60
1:C:63:ILE:HG12	3:C:506:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:MET:CB	1:A:41:PRO:CD	2.80	0.60
1:B:44:ARG:HA	3:C:505:HOH:O	2.00	0.60
1:A:77:LEU:HD21	1:A:308:MET:HE1	1.84	0.59
1:C:73:ASN:HB3	1:C:308:MET:SD	2.43	0.59
1:B:166:TYR:CE2	3:B:573:HOH:O	2.49	0.59
1:B:60:ASP:HB3	3:B:540:HOH:O	2.00	0.59
1:C:226:LEU:HD13	3:C:587:HOH:O	2.02	0.59
1:C:154:PRO:O	1:C:157:GLY:N	2.34	0.59
1:A:324:VAL:HG12	1:B:324:VAL:HG12	1.83	0.59
1:B:100:LEU:HB2	3:B:575:HOH:O	2.03	0.59
1:B:166:TYR:CE1	3:B:573:HOH:O	2.54	0.58
1:C:351:GLN:HG3	1:C:355:ASP:OD2	2.03	0.58
1:A:363:ALA:HB1	1:D:297:ASN:ND2	2.18	0.58
1:C:186:CYS:O	3:C:508:HOH:O	2.16	0.58
1:D:348:GLU:OE1	1:D:348:GLU:HA	2.04	0.57
1:D:254:LEU:CD2	3:D:524:HOH:O	2.52	0.57
1:A:38:THR:HA	3:A:528:HOH:O	2.03	0.57
1:A:131:LYS:HB3	3:A:579:HOH:O	2.04	0.57
1:A:290:ILE:HG22	1:A:304:MET:HE1	1.85	0.57
1:C:44:ARG:HD3	1:C:281:PHE:CE1	2.39	0.57
1:C:354:LEU:HD23	3:C:596:HOH:O	2.05	0.57
1:B:19:TYR:O	1:B:323:ALA:HA	2.05	0.57
1:C:40:MET:CB	1:C:41:PRO:CD	2.83	0.57
1:C:314:THR:HG23	3:C:550:HOH:O	2.05	0.57
1:D:291:TYR:CE1	1:D:302:LEU:HD23	2.40	0.57
1:C:226:LEU:CD1	3:C:587:HOH:O	2.53	0.56
1:D:156:PRO:C	3:D:535:HOH:O	2.48	0.56
1:D:294:VAL:HG23	3:D:569:HOH:O	2.03	0.56
1:A:162:HIS:HA	3:A:630:HOH:O	2.05	0.56
1:B:94:THR:HB	3:B:536:HOH:O	2.05	0.56
1:B:250:LEU:HD12	3:B:554:HOH:O	2.05	0.56
1:B:217:TYR:HB3	1:B:218:PRO:HD3	1.88	0.56
1:B:353:ILE:HG21	3:C:508:HOH:O	2.05	0.56
1:B:94:THR:HG21	1:C:101:VAL:HG22	1.87	0.55
1:A:19:TYR:O	1:A:323:ALA:HA	2.07	0.55
1:D:131:LYS:HD2	3:D:622:HOH:O	2.06	0.55
1:A:75:GLN:NE2	3:A:516:HOH:O	2.37	0.55
1:C:226:LEU:HB2	1:C:313:ILE:HD11	1.87	0.54
1:B:135:GLU:OE1	3:B:508:HOH:O	2.18	0.54
1:C:260:ALA:CB	3:C:532:HOH:O	2.49	0.54
3:B:519:HOH:O	1:C:215:ILE:CG2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ASN:O	1:C:85:THR:HG23	2.07	0.54
1:D:160:ASN:HA	3:D:577:HOH:O	2.07	0.54
1:C:324:VAL:HG21	3:D:523:HOH:O	2.08	0.54
1:A:16:ARG:NH2	3:A:523:HOH:O	2.39	0.54
1:A:110:ALA:HB1	1:A:331:ASP:OD2	2.07	0.53
1:A:259:SER:HA	3:A:532:HOH:O	2.07	0.53
1:C:274:HIS:CD2	3:C:587:HOH:O	2.61	0.53
1:C:288:TYR:N	3:C:514:HOH:O	2.31	0.53
1:C:282:ASN:OD1	1:C:287:ARG:NE	2.39	0.53
1:B:220:TYR:O	3:B:509:HOH:O	2.19	0.53
1:D:132:TYR:O	1:D:135:GLU:HB3	2.08	0.53
1:D:108:TRP:CD2	3:D:535:HOH:O	2.53	0.53
1:D:40:MET:CB	1:D:41:PRO:HD2	2.29	0.53
1:C:279:ALA:HB3	3:C:529:HOH:O	2.09	0.53
1:D:71:MET:HE3	3:D:514:HOH:O	2.08	0.53
1:A:360:VAL:O	1:A:364:ASN:ND2	2.41	0.53
1:D:34:ILE:HG23	3:D:526:HOH:O	2.09	0.53
1:B:189:ALA:HB1	1:C:147:THR:HB	1.91	0.52
1:C:213:PRO:HG3	3:C:627:HOH:O	2.08	0.52
1:A:13:ALA:O	1:A:16:ARG:NH1	2.43	0.52
1:C:217:TYR:HB3	1:C:218:PRO:HD3	1.92	0.52
1:B:88:PHE:HE2	3:B:614:HOH:O	1.92	0.52
1:C:213:PRO:HA	3:C:602:HOH:O	2.10	0.52
1:C:270:VAL:HA	3:C:518:HOH:O	2.09	0.52
1:A:161:VAL:HG23	3:A:547:HOH:O	2.09	0.52
1:B:40:MET:HB2	1:B:41:PRO:HD3	1.86	0.52
1:B:136:HIS:CE1	3:B:531:HOH:O	2.63	0.52
1:D:233:MET:HG3	3:D:599:HOH:O	2.09	0.51
1:B:362:GLU:H	1:B:362:GLU:CD	2.17	0.51
1:B:174:TYR:HB3	1:B:181:PHE:HB2	1.93	0.51
1:D:107:GLY:HA2	1:D:110:ALA:HB3	1.92	0.51
1:A:372:MET:HE3	1:D:250:LEU:HD21	1.92	0.51
1:B:19:TYR:HB3	1:B:310:VAL:HG11	1.91	0.51
1:B:98:GLY:HA3	3:B:536:HOH:O	2.11	0.51
1:C:184:TRP:HZ2	3:C:608:HOH:O	1.93	0.51
1:D:304:MET:CE	3:D:615:HOH:O	2.58	0.51
1:B:40:MET:CB	1:B:41:PRO:HD2	2.35	0.51
1:C:64:VAL:HG21	1:C:207:PHE:CE2	2.45	0.51
1:C:279:ALA:CB	3:C:529:HOH:O	2.57	0.51
1:B:63:ILE:HD11	1:B:84:LEU:HB3	1.92	0.51
1:C:164:PHE:HA	3:C:575:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:GLN:O	1:C:355:ASP:OD2	2.28	0.51
1:C:20:TYR:CD1	1:D:20:TYR:CD1	2.99	0.51
1:A:20:TYR:CD1	1:B:20:TYR:CD1	2.99	0.51
1:B:21:PRO:HG2	1:B:325:SER:HB3	1.92	0.51
1:B:254:LEU:CD2	3:B:554:HOH:O	2.59	0.51
1:C:359:ASN:OD1	1:C:361:ASP:OD2	2.28	0.51
1:B:332:VAL:HB	3:B:628:HOH:O	2.11	0.50
1:A:142:ASN:CB	3:D:513:HOH:O	2.60	0.50
1:D:214:ASN:CB	3:D:588:HOH:O	2.41	0.50
1:A:34:ILE:HD13	1:A:77:LEU:HD22	1.94	0.50
1:D:67:GLY:O	1:D:70:SER:OG	2.17	0.50
1:D:127:ASP:HB2	3:D:513:HOH:O	2.12	0.50
1:B:31:ILE:HG22	1:B:313:ILE:HD12	1.94	0.50
1:D:280:PHE:O	3:D:502:HOH:O	2.19	0.50
1:A:174:TYR:HB3	1:A:181:PHE:HB2	1.93	0.50
1:C:18:VAL:HG22	1:D:78:MET:HE1	1.92	0.49
1:D:117:GLU:OE1	1:D:162:HIS:NE2	2.45	0.49
1:C:39:GLY:O	1:C:40:MET:SD	2.70	0.49
1:D:141:TYR:O	1:D:144:ASP:HB3	2.11	0.49
1:B:266:ILE:O	1:B:270:VAL:HG23	2.12	0.49
1:A:142:ASN:HB3	3:D:513:HOH:O	2.12	0.49
1:B:31:ILE:CG2	1:B:313:ILE:HD12	2.42	0.49
1:D:83:TYR:C	3:D:512:HOH:O	2.56	0.49
1:B:101:VAL:HG11	3:B:551:HOH:O	2.11	0.49
1:C:154:PRO:CB	3:C:613:HOH:O	2.50	0.49
1:A:104:TRP:CD1	1:A:159:ILE:HD11	2.48	0.49
1:D:131:LYS:HE3	1:D:161:VAL:HB	1.93	0.49
1:C:116:LEU:HD21	3:C:558:HOH:O	2.12	0.48
1:C:244:GLN:HA	1:C:244:GLN:HE21	1.78	0.48
1:A:208:GLY:N	1:A:228:ILE:O	2.46	0.48
1:D:156:PRO:HB2	3:D:535:HOH:O	2.12	0.48
1:D:187:ILE:CD1	3:D:588:HOH:O	2.57	0.48
1:B:198:LEU:HD23	1:B:198:LEU:C	2.38	0.48
1:A:41:PRO:HA	1:A:95:ASP:OD2	2.13	0.48
1:B:110:ALA:HA	3:B:539:HOH:O	2.13	0.48
1:D:290:ILE:HB	3:D:615:HOH:O	2.14	0.48
1:B:66:ILE:HG23	1:B:66:ILE:O	2.14	0.48
1:B:194:VAL:N	3:B:513:HOH:O	2.47	0.48
1:C:240:THR:HA	3:C:554:HOH:O	2.13	0.48
1:A:45:ARG:NH2	1:D:325:SER:OG	2.42	0.48
1:B:263:PHE:CE2	1:B:267:MET:HE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:TYR:HB2	1:B:304:MET:HE2	1.95	0.48
1:B:143:TRP:HB2	3:B:546:HOH:O	2.13	0.48
1:B:356:GLY:HA3	1:C:216:TRP:CH2	2.49	0.48
1:C:16:ARG:HA	3:C:626:HOH:O	2.13	0.48
1:C:285:ASP:OD1	1:C:286:THR:HG23	2.13	0.47
1:D:246:ALA:HB3	3:D:603:HOH:O	2.14	0.47
1:D:34:ILE:HG12	3:D:629:HOH:O	2.14	0.47
1:C:52:TRP:CZ2	1:C:228:ILE:HG21	2.49	0.47
1:C:155:ARG:HB3	1:C:156:PRO:HD3	1.95	0.47
1:D:150:VAL:HG12	1:D:151:THR:HG23	1.95	0.47
1:A:40:MET:CG	1:A:41:PRO:HD3	2.45	0.47
1:A:367:TRP:CH2	3:D:524:HOH:O	2.56	0.47
1:B:323:ALA:HB2	3:B:593:HOH:O	2.14	0.47
1:B:62:PHE:CE2	3:B:540:HOH:O	2.67	0.47
1:C:156:PRO:HB2	3:C:525:HOH:O	2.14	0.47
1:D:24:GLU:OE2	3:D:503:HOH:O	2.21	0.47
1:A:73:ASN:HB3	1:A:308:MET:SD	2.54	0.47
1:B:181:PHE:CZ	1:B:198:LEU:HD12	2.49	0.47
1:A:44:ARG:HD2	1:A:281:PHE:CE1	2.50	0.47
1:A:303:SER:OG	1:A:320:GLU:OE1	2.29	0.47
1:D:233:MET:CG	3:D:599:HOH:O	2.48	0.47
1:B:313:ILE:HD13	3:B:537:HOH:O	2.14	0.47
1:C:310:VAL:CG1	1:C:321:ARG:HB2	2.44	0.47
1:D:174:TYR:HB3	1:D:181:PHE:HB2	1.95	0.47
1:A:217:TYR:HB3	1:A:218:PRO:HD3	1.95	0.46
1:D:250:LEU:HG	3:D:524:HOH:O	2.14	0.46
1:D:149:ALA:O	1:D:150:VAL:C	2.58	0.46
1:A:313:ILE:C	3:A:552:HOH:O	2.58	0.46
1:C:359:ASN:ND2	1:C:362:GLU:OE1	2.48	0.46
1:D:217:TYR:HB3	1:D:218:PRO:HD3	1.97	0.46
1:D:323:ALA:HB2	3:D:526:HOH:O	2.14	0.46
1:A:43:ALA:HB3	3:D:514:HOH:O	2.15	0.46
1:C:295:ARG:NH2	1:C:300:GLY:O	2.49	0.46
1:C:193:PRO:CG	3:C:600:HOH:O	2.63	0.46
1:C:286:THR:C	3:C:514:HOH:O	2.59	0.46
1:B:132:TYR:HB2	3:B:559:HOH:O	2.15	0.46
1:B:137:MET:O	1:B:140:ALA:HB3	2.16	0.46
1:C:96:HIS:NE2	3:C:501:HOH:O	2.36	0.46
1:C:262:SER:CB	3:C:627:HOH:O	2.61	0.46
1:D:155:ARG:HB3	1:D:156:PRO:HD3	1.98	0.46
1:A:231:CYS:CB	1:A:277:ALA:HB1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:MET:HE1	1:B:233:MET:HE3	1.98	0.46
1:C:20:TYR:HB3	1:D:20:TYR:CD2	2.51	0.46
1:C:225:ASP:O	1:C:273:ARG:HB2	2.16	0.46
1:C:295:ARG:O	1:C:296:GLU:C	2.59	0.46
1:A:141:TYR:HA	3:D:560:HOH:O	2.16	0.45
3:A:582:HOH:O	1:D:141:TYR:HA	2.16	0.45
1:B:39:GLY:O	1:B:40:MET:O	2.34	0.45
1:C:310:VAL:HG13	1:C:321:ARG:HB2	1.98	0.45
1:B:134:VAL:HG11	1:B:161:VAL:HG22	1.97	0.45
1:D:27:GLY:O	1:D:57:GLY:HA2	2.16	0.45
1:A:233:MET:HE2	1:A:237:GLN:HB3	1.98	0.45
1:A:280:PHE:CZ	1:A:304:MET:HE3	2.51	0.45
1:B:121:PRO:HB3	3:B:513:HOH:O	2.16	0.45
1:C:19:TYR:O	1:C:323:ALA:HA	2.17	0.45
1:A:345:ARG:NH1	3:A:537:HOH:O	2.48	0.45
1:B:288:TYR:HB3	1:D:291:TYR:CZ	2.51	0.45
1:A:295:ARG:NH2	1:A:300:GLY:O	2.39	0.45
1:B:360:VAL:O	1:B:364:ASN:ND2	2.49	0.45
1:C:91:HIS:HB3	1:C:193:PRO:HA	1.98	0.45
1:C:225:ASP:HA	1:C:273:ARG:HB2	1.99	0.45
1:D:253:ASN:O	1:D:259:SER:HB3	2.16	0.45
1:B:89:LEU:HD22	1:B:97:TRP:HB3	1.98	0.45
1:C:186:CYS:HB2	1:C:193:PRO:HB2	1.97	0.45
1:D:40:MET:CB	1:D:41:PRO:CD	2.82	0.45
1:C:274:HIS:CG	3:C:587:HOH:O	2.69	0.45
1:D:91:HIS:CD2	1:D:93:HIS:ND1	2.85	0.45
1:C:359:ASN:OD1	1:C:361:ASP:CG	2.59	0.45
1:A:44:ARG:HB3	1:D:329:ALA:HB3	1.99	0.45
1:B:142:ASN:ND2	1:C:127:ASP:O	2.50	0.44
1:D:48:ALA:N	1:D:307:ASP:OD2	2.43	0.44
1:C:156:PRO:CB	3:C:525:HOH:O	2.66	0.44
1:B:127:ASP:OD1	1:B:127:ASP:C	2.60	0.44
1:A:145:TYR:O	3:A:504:HOH:O	2.21	0.44
1:B:231:CYS:SG	1:B:260:ALA:HA	2.57	0.44
1:C:63:ILE:CD1	1:C:103:MET:HE3	2.48	0.44
1:A:16:ARG:CZ	3:A:523:HOH:O	2.65	0.44
1:A:231:CYS:HB3	1:A:277:ALA:HB1	2.00	0.44
3:B:548:HOH:O	1:C:190:GLY:C	2.59	0.44
1:C:102:SER:O	1:C:106:GLY:N	2.39	0.44
1:C:366:HIS:CD2	3:C:619:HOH:O	2.71	0.44
1:D:187:ILE:CG1	3:D:588:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:O	1:A:238:MET:HB2	2.17	0.44
1:C:181:PHE:CZ	1:C:198:LEU:HD12	2.53	0.44
1:D:217:TYR:CE1	1:D:221:ALA:CB	2.99	0.44
1:B:19:TYR:HB2	1:B:310:VAL:HG11	1.99	0.44
1:C:144:ASP:OD1	1:C:148:ARG:NH1	2.50	0.44
1:D:120:GLY:HA3	1:D:130:THR:HG21	1.99	0.44
1:B:61:LYS:HE3	3:B:604:HOH:O	2.17	0.44
1:B:78:MET:HA	3:B:628:HOH:O	2.17	0.44
1:C:120:GLY:O	3:C:509:HOH:O	2.20	0.44
1:B:210:ASP:CG	3:B:505:HOH:O	2.59	0.43
1:B:214:ASN:ND2	3:B:535:HOH:O	2.50	0.43
1:D:105:ALA:O	1:D:109:THR:HG23	2.18	0.43
1:A:278:TYR:O	1:A:279:ALA:HB3	2.18	0.43
1:B:42:THR:CG2	3:C:519:HOH:O	2.65	0.43
1:D:206:VAL:HG11	1:D:217:TYR:CZ	2.53	0.43
1:B:21:PRO:HB3	1:B:77:LEU:HA	2.01	0.43
1:C:66:ILE:HG23	1:C:66:ILE:O	2.19	0.43
1:C:137:MET:O	1:C:140:ALA:HB3	2.18	0.43
1:B:14:PRO:O	1:B:15:LYS:C	2.62	0.43
1:B:40:MET:HE1	1:B:233:MET:CE	2.48	0.43
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.91	0.43
1:B:237:GLN:HB3	3:B:608:HOH:O	2.17	0.43
1:C:145:TYR:CD1	1:C:145:TYR:C	2.96	0.43
1:C:253:ASN:HA	3:C:573:HOH:O	2.19	0.43
1:D:198:LEU:C	1:D:198:LEU:HD23	2.43	0.43
1:C:186:CYS:SG	1:C:211:THR:HB	2.59	0.43
3:A:508:HOH:O	1:D:42:THR:HG22	2.17	0.43
1:B:226:LEU:N	3:B:537:HOH:O	2.52	0.43
1:B:94:THR:HG22	1:C:141:TYR:CE1	2.52	0.43
1:D:34:ILE:HD13	1:D:77:LEU:HD13	2.00	0.43
1:A:40:MET:CG	1:A:41:PRO:CD	2.97	0.42
1:A:66:ILE:CG1	1:A:66:ILE:O	2.65	0.42
1:B:313:ILE:HG23	1:B:318:VAL:HG22	2.00	0.42
1:C:226:LEU:CB	1:C:313:ILE:HD11	2.49	0.42
1:D:33:VAL:O	1:D:310:VAL:HA	2.19	0.42
1:D:97:TRP:O	1:D:100:LEU:N	2.52	0.42
1:A:108:TRP:CE3	1:A:148:ARG:HD2	2.54	0.42
1:B:273:ARG:HB3	3:B:578:HOH:O	2.19	0.42
1:C:362:GLU:CD	1:C:362:GLU:H	2.27	0.42
1:D:106:GLY:O	1:D:109:THR:N	2.52	0.42
1:D:290:ILE:O	1:D:294:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CE2	3:A:596:HOH:O	2.71	0.42
1:D:47:GLN:HA	1:D:307:ASP:CG	2.44	0.42
1:D:238:MET:HE2	1:D:252:ILE:HD13	2.01	0.42
1:A:348:GLU:N	3:A:526:HOH:O	2.42	0.42
1:A:356:GLY:HA3	1:D:216:TRP:CH2	2.54	0.42
1:B:181:PHE:CE1	1:B:198:LEU:HG	2.54	0.42
1:C:40:MET:HB2	1:C:41:PRO:CD	2.50	0.42
1:C:351:GLN:HE21	1:C:355:ASP:CG	2.28	0.42
1:D:352:TYR:O	1:D:352:TYR:CD1	2.72	0.42
1:A:69:GLY:N	1:A:99:ASP:OD2	2.53	0.42
1:A:33:VAL:O	1:A:310:VAL:HA	2.19	0.42
1:B:291:TYR:HD2	3:B:514:HOH:O	2.01	0.42
1:C:307:ASP:O	1:C:322:MET:HE1	2.19	0.42
1:D:66:ILE:HG23	1:D:66:ILE:O	2.19	0.42
1:A:118:VAL:CG1	3:A:554:HOH:O	2.67	0.42
1:A:185:PRO:HB2	1:A:216:TRP:CZ3	2.55	0.42
1:A:204:LYS:NZ	3:A:527:HOH:O	2.43	0.42
1:B:34:ILE:HD13	1:B:77:LEU:HD22	2.02	0.42
1:B:128:MET:HB3	3:C:599:HOH:O	2.19	0.42
1:C:54:VAL:HG21	1:C:207:PHE:HZ	1.84	0.42
1:D:190:GLY:O	1:D:191:ASP:C	2.63	0.42
1:B:330:TRP:CZ3	1:C:241:LYS:HG3	2.54	0.42
1:D:101:VAL:HG21	1:D:141:TYR:CE2	2.55	0.42
1:D:254:LEU:HD23	3:D:524:HOH:O	2.18	0.42
1:A:234:THR:O	1:A:237:GLN:N	2.51	0.42
1:A:367:TRP:O	1:A:367:TRP:CE3	2.72	0.42
1:C:18:VAL:HG21	3:D:523:HOH:O	2.19	0.41
1:C:290:ILE:HG22	1:C:304:MET:HE1	2.02	0.41
1:A:31:ILE:CG2	1:A:313:ILE:HD12	2.50	0.41
1:A:66:ILE:O	1:A:66:ILE:HG12	2.19	0.41
1:B:90:THR:O	1:B:91:HIS:HB3	2.20	0.41
1:C:40:MET:HE3	1:C:40:MET:HA	2.03	0.41
1:C:329:ALA:C	3:C:519:HOH:O	2.64	0.41
1:C:354:LEU:CD2	3:C:596:HOH:O	2.67	0.41
1:A:37:GLY:O	1:A:50:ALA:HA	2.20	0.41
1:A:104:TRP:HA	1:A:116:LEU:HD11	2.02	0.41
1:A:109:THR:O	1:A:111:GLY:N	2.53	0.41
1:B:261:GLN:O	1:B:297:ASN:ND2	2.53	0.41
1:B:241:LYS:HE3	3:B:632:HOH:O	2.20	0.41
1:B:308:MET:HE2	1:B:325:SER:OG	2.21	0.41
1:D:108:TRP:CG	3:D:535:HOH:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ALA:HB3	1:C:270:VAL:HG22	2.02	0.41
1:A:175:GLN:NE2	3:A:549:HOH:O	2.54	0.41
1:A:20:TYR:HB3	1:B:20:TYR:CG	2.56	0.41
1:A:288:TYR:O	1:A:291:TYR:HB3	2.21	0.41
1:D:247:GLN:HA	3:D:585:HOH:O	2.20	0.41
1:A:14:PRO:O	1:A:15:LYS:C	2.63	0.41
1:A:20:TYR:HE2	1:B:21:PRO:O	2.04	0.41
1:A:105:ALA:HB1	1:A:148:ARG:HH12	1.84	0.41
1:A:212:ALA:O	1:A:213:PRO:C	2.64	0.41
1:B:139:LYS:HD3	1:C:132:TYR:OH	2.20	0.41
3:B:506:HOH:O	1:C:350:THR:CG2	2.58	0.41
1:A:91:HIS:HE1	1:A:96:HIS:CE1	2.39	0.41
1:C:8:SER:OG	1:C:11:GLY:HA3	2.21	0.41
1:C:58:ASN:OD1	1:C:59:GLY:N	2.54	0.41
1:D:178:GLY:O	1:D:200:TRP:HD1	2.04	0.41
1:A:175:GLN:NE2	1:A:180:THR:HG23	2.36	0.40
1:B:226:LEU:CB	3:B:537:HOH:O	2.69	0.40
1:B:271:GLN:CB	3:B:589:HOH:O	2.69	0.40
1:C:326:PRO:HG3	1:D:18:VAL:HG21	2.03	0.40
1:D:216:TRP:O	1:D:217:TYR:C	2.64	0.40
1:A:263:PHE:CD1	1:A:263:PHE:C	2.99	0.40
1:B:133:ALA:HB3	3:B:533:HOH:O	2.21	0.40
1:A:109:THR:C	1:A:111:GLY:N	2.79	0.40
1:A:221:ALA:O	1:A:222:LYS:C	2.65	0.40
1:A:312:ASN:ND2	3:A:541:HOH:O	2.49	0.40
1:D:362:GLU:OE1	1:D:363:ALA:N	2.36	0.40
1:A:155:ARG:HB3	1:A:156:PRO:HD3	2.04	0.40
1:B:238:MET:HE2	1:B:252:ILE:HD13	2.03	0.40
1:C:88:PHE:HZ	3:C:610:HOH:O	1.87	0.40
1:D:93:HIS:CE1	1:D:188:HIS:NE2	2.90	0.40
1:D:187:ILE:HG13	3:D:588:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/372 (96%)	319 (89%)	30 (8%)	9 (2%)	4	1
1	B	356/372 (96%)	315 (88%)	37 (10%)	4 (1%)	11	4
1	C	356/372 (96%)	310 (87%)	40 (11%)	6 (2%)	7	2
1	D	358/372 (96%)	316 (88%)	30 (8%)	12 (3%)	3	0
All	All	1428/1488 (96%)	1260 (88%)	137 (10%)	31 (2%)	5	1

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	B	40	MET
1	C	40	MET
1	D	65	ASP
1	D	150	VAL
1	A	110	ALA
1	A	222	LYS
1	A	279	ALA
1	C	35	ALA
1	C	222	LYS
1	D	98	GLY
1	D	188	HIS
1	D	362	GLU
1	A	50	ALA
1	A	211	THR
1	B	91	HIS
1	C	44	ARG
1	D	66	ILE
1	D	200	TRP
1	C	282	ASN
1	D	240	THR
1	B	279	ALA
1	D	40	MET
1	D	363	ALA
1	C	233	MET
1	D	308	MET
1	A	41	PRO
1	B	111	GLY
1	A	66	ILE
1	A	106	GLY

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Mol	Chain	Res	Type
1	D	106	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/301 (97%)	280 (96%)	12 (4%)	27	17
1	B	288/301 (96%)	271 (94%)	17 (6%)	18	7
1	C	288/301 (96%)	277 (96%)	11 (4%)	29	19
1	D	292/301 (97%)	281 (96%)	11 (4%)	29	19
All	All	1160/1204 (96%)	1109 (96%)	51 (4%)	25	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	A	42	THR
1	A	117	GLU
1	A	158	ASP
1	A	169	LEU
1	A	199	GLU
1	A	248	LEU
1	A	295	ARG
1	A	306	THR
1	A	331	ASP
1	A	362	GLU
1	A	372	MET
1	B	15	LYS
1	B	40	MET
1	B	101	VAL
1	B	114	ASP
1	B	131	LYS
1	B	161	VAL
1	B	169	LEU
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	222	LYS
1	B	254	LEU
1	B	255	ASP
1	B	258	THR
1	B	281	PHE
1	B	297	ASN
1	B	331	ASP
1	B	347	SER
1	B	362	GLU
1	C	25	GLU
1	C	40	MET
1	C	93	HIS
1	C	117	GLU
1	C	180	THR
1	C	195	SER
1	C	233	MET
1	C	253	ASN
1	C	254	LEU
1	C	319	THR
1	C	362	GLU
1	D	109	THR
1	D	131	LYS
1	D	191	ASP
1	D	199	GLU
1	D	254	LEU
1	D	295	ARG
1	D	310	VAL
1	D	331	ASP
1	D	347	SER
1	D	362	GLU
1	D	368	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	237	GLN
1	A	257	HIS
1	B	142	ASN
1	B	162	HIS
1	B	170	ASN
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	243	ASN
1	B	364	ASN
1	C	75	GLN
1	C	153	ASN
1	C	177	ASN
1	C	244	GLN
1	C	297	ASN
1	C	351	GLN
1	C	366	HIS
1	D	75	GLN
1	D	82	ASN
1	D	244	GLN
1	D	257	HIS
1	D	265	GLN
1	D	297	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/372 (97%)	3.37	256 (70%) 0 0	6, 17, 41, 51	0
1	B	360/372 (96%)	3.91	296 (82%) 0 0	5, 20, 46, 58	0
1	C	360/372 (96%)	4.72	341 (94%) 0 0	13, 25, 41, 58	0
1	D	362/372 (97%)	4.09	308 (85%) 0 0	2, 21, 38, 60	0
All	All	1444/1488 (97%)	4.02	1201 (83%) 0 0	2, 21, 41, 60	0

All (1201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	16.2
1	C	368	LYS	14.5
1	D	248	LEU	13.8
1	A	360	VAL	13.5
1	C	8	SER	13.1
1	D	246	ALA	13.1
1	B	152	ILE	12.6
1	D	245	PRO	12.3
1	C	365	ALA	12.0
1	B	365	ALA	11.7
1	B	240	THR	11.1
1	B	371	PHE	11.1
1	C	110	ALA	11.0
1	B	373	GLY	10.8
1	C	366	HIS	10.8
1	B	242	TYR	10.8
1	B	360	VAL	10.6
1	D	13	ALA	10.6
1	C	249	ALA	10.4
1	B	245	PRO	10.4
1	A	8	SER	10.4

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Mol	Chain	Res	Type	RSRZ
1	D	254	LEU	10.4
1	D	249	ALA	10.3
1	D	368	LYS	10.3
1	A	358	LEU	10.1
1	C	203	TYR	10.1
1	D	372	MET	10.1
1	C	7	THR	10.0
1	A	250	LEU	10.0
1	C	5	LYS	9.9
1	B	367	TRP	9.9
1	D	250	LEU	9.8
1	B	250	LEU	9.8
1	A	241	LYS	9.8
1	A	251	ARG	9.8
1	A	249	ALA	9.7
1	C	108	TRP	9.7
1	B	8	SER	9.7
1	C	113	THR	9.7
1	B	243	ASN	9.6
1	C	367	TRP	9.6
1	B	241	LYS	9.5
1	A	363	ALA	9.5
1	C	248	LEU	9.5
1	D	243	ASN	9.5
1	D	294	VAL	9.5
1	D	150	VAL	9.4
1	A	252	ILE	9.4
1	A	246	ALA	9.4
1	D	242	TYR	9.4
1	C	263	PHE	9.3
1	C	246	ALA	9.3
1	D	365	ALA	9.3
1	C	250	LEU	9.3
1	B	6	VAL	9.3
1	D	215	ILE	9.2
1	D	251	ARG	9.2
1	A	2	ALA	9.2
1	D	151	THR	9.2
1	D	373	GLY	9.1
1	B	244	GLN	9.1
1	D	154	PRO	9.0
1	B	9	SER	9.0

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Mol	Chain	Res	Type	RSRZ
1	D	369	GLN	8.9
1	D	240	THR	8.9
1	D	212	ALA	8.8
1	D	11	GLY	8.8
1	B	254	LEU	8.8
1	B	249	ALA	8.8
1	B	2	ALA	8.7
1	C	242	TYR	8.7
1	B	111	GLY	8.6
1	D	367	TRP	8.6
1	C	151	THR	8.6
1	C	14	PRO	8.5
1	D	329	ALA	8.5
1	B	256	PHE	8.5
1	A	245	PRO	8.4
1	C	266	ILE	8.3
1	C	114	ASP	8.3
1	D	371	PHE	8.3
1	B	7	THR	8.3
1	C	6	VAL	8.3
1	B	353	ILE	8.2
1	A	365	ALA	8.2
1	B	330	TRP	8.2
1	A	371	PHE	8.2
1	B	363	ALA	8.1
1	D	6	VAL	8.1
1	B	5	LYS	8.0
1	C	116	LEU	8.0
1	D	253	ASN	8.0
1	C	360	VAL	8.0
1	D	187	ILE	8.0
1	B	372	MET	7.9
1	D	110	ALA	7.9
1	C	13	ALA	7.9
1	B	352	TYR	7.9
1	C	284	ASP	7.7
1	C	372	MET	7.7
1	D	252	ILE	7.7
1	D	7	THR	7.7
1	D	314	THR	7.7
1	C	298	TYR	7.7
1	D	244	GLN	7.6

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Mol	Chain	Res	Type	RSRZ
1	C	371	PHE	7.6
1	C	294	VAL	7.6
1	C	216	TRP	7.6
1	B	187	ILE	7.6
1	A	367	TRP	7.6
1	B	333	ALA	7.6
1	A	373	GLY	7.5
1	C	233	MET	7.5
1	B	252	ILE	7.5
1	D	12	ILE	7.5
1	B	110	ALA	7.5
1	D	152	ILE	7.4
1	B	13	ALA	7.4
1	C	237	GLN	7.4
1	C	369	GLN	7.4
1	B	255	ASP	7.4
1	C	115	PRO	7.4
1	C	239	MET	7.3
1	A	7	THR	7.3
1	B	232	TRP	7.3
1	A	354	LEU	7.3
1	C	240	THR	7.3
1	A	232	TRP	7.2
1	C	149	ALA	7.2
1	A	110	ALA	7.2
1	A	372	MET	7.2
1	B	366	HIS	7.2
1	D	247	GLN	7.2
1	A	209	GLY	7.1
1	B	263	PHE	7.1
1	B	354	LEU	7.1
1	D	108	TRP	7.1
1	B	246	ALA	7.1
1	C	109	THR	7.0
1	C	183	SER	7.0
1	C	198	LEU	7.0
1	B	3	GLY	7.0
1	C	159	ILE	7.0
1	C	150	VAL	7.0
1	C	92	LEU	7.0
1	B	108	TRP	7.0
1	B	233	MET	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	185	PRO	7.0
1	C	184	TRP	7.0
1	B	14	PRO	6.9
1	A	238	MET	6.9
1	C	40	MET	6.9
1	D	101	VAL	6.9
1	D	9	SER	6.9
1	B	251	ARG	6.9
1	C	290	ILE	6.9
1	C	2	ALA	6.8
1	C	46	ALA	6.8
1	A	291	TYR	6.8
1	B	369	GLN	6.8
1	C	245	PRO	6.8
1	C	217	TYR	6.8
1	C	225	ASP	6.8
1	C	252	ILE	6.8
1	D	210	ASP	6.8
1	C	104	TRP	6.7
1	C	373	GLY	6.7
1	A	242	TYR	6.7
1	C	152	ILE	6.7
1	B	221	ALA	6.7
1	C	168	ALA	6.7
1	D	2	ALA	6.7
1	D	10	THR	6.7
1	A	254	LEU	6.7
1	C	247	GLN	6.7
1	C	256	PHE	6.7
1	B	288	TYR	6.7
1	B	12	ILE	6.7
1	C	270	VAL	6.6
1	C	243	ASN	6.6
1	D	147	THR	6.6
1	D	233	MET	6.6
1	C	292	THR	6.6
1	D	189	ALA	6.6
1	C	155	ARG	6.6
1	C	4	GLY	6.5
1	B	189	ALA	6.5
1	D	121	PRO	6.5
1	D	263	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	279	ALA	6.5
1	B	154	PRO	6.5
1	C	160	ASN	6.5
1	D	216	TRP	6.5
1	C	194	VAL	6.5
1	A	240	THR	6.4
1	D	100	LEU	6.4
1	C	318	VAL	6.4
1	A	288	TYR	6.4
1	A	352	TYR	6.4
1	D	226	LEU	6.4
1	A	356	GLY	6.4
1	B	109	THR	6.4
1	C	187	ILE	6.4
1	B	361	ASP	6.4
1	B	28	PRO	6.3
1	A	256	PHE	6.3
1	A	244	GLN	6.3
1	B	10	THR	6.3
1	C	238	MET	6.3
1	D	256	PHE	6.3
1	D	260	ALA	6.3
1	B	234	THR	6.2
1	B	370	GLU	6.2
1	D	217	TYR	6.2
1	D	8	SER	6.2
1	A	41	PRO	6.2
1	B	11	GLY	6.2
1	B	356	GLY	6.2
1	B	294	VAL	6.2
1	D	297	ASN	6.2
1	C	166	TYR	6.2
1	C	220	TYR	6.2
1	C	231	CYS	6.2
1	A	11	GLY	6.2
1	B	216	TRP	6.1
1	D	168	ALA	6.1
1	D	333	ALA	6.1
1	C	234	THR	6.1
1	D	366	HIS	6.1
1	B	105	ALA	6.1
1	A	359	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	226	LEU	6.1
1	C	358	LEU	6.1
1	B	266	ILE	6.1
1	C	224	ALA	6.1
1	A	243	ASN	6.1
1	C	26	LEU	6.1
1	D	370	GLU	6.0
1	D	346	ALA	6.0
1	C	232	TRP	6.0
1	B	39	GLY	6.0
1	D	335	PRO	6.0
1	C	200	TRP	6.0
1	A	28	PRO	6.0
1	B	116	LEU	6.0
1	B	121	PRO	6.0
1	D	313	ILE	6.0
1	B	211	THR	6.0
1	C	363	ALA	6.0
1	D	363	ALA	6.0
1	B	332	VAL	6.0
1	D	41	PRO	6.0
1	B	358	LEU	6.0
1	C	353	ILE	6.0
1	B	357	ARG	5.9
1	C	122	SER	5.9
1	C	133	ALA	5.9
1	C	154	PRO	5.9
1	C	215	ILE	5.9
1	C	3	GLY	5.9
1	C	359	ASN	5.9
1	C	236	ASP	5.9
1	A	150	VAL	5.9
1	C	169	LEU	5.9
1	D	358	LEU	5.9
1	A	369	GLN	5.8
1	B	368	LYS	5.8
1	B	150	VAL	5.8
1	A	370	GLU	5.8
1	C	12	ILE	5.8
1	C	209	GLY	5.8
1	A	213	PRO	5.8
1	D	173	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	5.8
1	D	239	MET	5.8
1	B	212	ALA	5.8
1	C	181	PHE	5.8
1	C	167	ARG	5.7
1	C	255	ASP	5.7
1	D	318	VAL	5.7
1	C	111	GLY	5.7
1	C	212	ALA	5.7
1	A	109	THR	5.7
1	C	118	VAL	5.7
1	C	106	GLY	5.7
1	A	235	SER	5.7
1	A	113	THR	5.6
1	D	241	LYS	5.6
1	A	366	HIS	5.6
1	C	352	TYR	5.6
1	C	197	ALA	5.6
1	D	207	PHE	5.6
1	B	235	SER	5.6
1	C	235	SER	5.6
1	D	291	TYR	5.6
1	C	153	ASN	5.6
1	C	147	THR	5.6
1	A	239	MET	5.5
1	C	262	SER	5.5
1	A	211	THR	5.5
1	C	319	THR	5.5
1	A	158	ASP	5.5
1	D	116	LEU	5.5
1	B	213	PRO	5.5
1	A	355	ASP	5.5
1	D	266	ILE	5.5
1	B	62	PHE	5.5
1	C	196	PHE	5.5
1	B	41	PRO	5.4
1	B	218	PRO	5.4
1	D	213	PRO	5.4
1	D	232	TRP	5.4
1	C	349	TYR	5.4
1	D	167	ARG	5.4
1	C	143	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	122	SER	5.4
1	A	368	LYS	5.4
1	C	329	ALA	5.4
1	A	6	VAL	5.4
1	A	216	TRP	5.4
1	A	350	THR	5.4
1	C	210	ASP	5.4
1	D	111	GLY	5.4
1	D	315	ARG	5.4
1	D	109	THR	5.3
1	B	217	TYR	5.3
1	C	291	TYR	5.3
1	A	69	GLY	5.3
1	C	164	PHE	5.3
1	D	295	ARG	5.3
1	C	107	GLY	5.3
1	C	274	HIS	5.3
1	A	319	THR	5.3
1	A	329	ALA	5.3
1	C	105	ALA	5.3
1	D	234	THR	5.3
1	D	258	THR	5.3
1	A	361	ASP	5.3
1	A	353	ILE	5.3
1	B	248	LEU	5.3
1	C	42	THR	5.3
1	C	260	ALA	5.3
1	C	357	ARG	5.3
1	C	202	GLY	5.2
1	A	52	TRP	5.2
1	C	280	PHE	5.2
1	D	211	THR	5.2
1	B	169	LEU	5.2
1	B	364	ASN	5.2
1	C	172	VAL	5.2
1	A	4	GLY	5.2
1	C	264	GLY	5.2
1	A	217	TYR	5.2
1	C	174	TYR	5.2
1	C	285	ASP	5.2
1	C	277	ALA	5.2
1	D	172	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	360	VAL	5.2
1	C	228	ILE	5.2
1	B	220	TYR	5.2
1	D	169	LEU	5.2
1	C	41	PRO	5.1
1	C	38	THR	5.1
1	C	211	THR	5.1
1	D	126	GLU	5.1
1	D	188	HIS	5.1
1	D	257	HIS	5.1
1	B	200	TRP	5.1
1	A	154	PRO	5.1
1	B	215	ILE	5.1
1	D	214	ASN	5.1
1	D	228	ILE	5.1
1	A	151	THR	5.1
1	A	351	GLN	5.1
1	C	193	PRO	5.1
1	B	153	ASN	5.1
1	A	12	ILE	5.1
1	D	319	THR	5.1
1	C	278	TYR	5.1
1	B	173	VAL	5.1
1	A	143	TRP	5.1
1	D	35	ALA	5.0
1	A	26	LEU	5.0
1	A	332	VAL	5.0
1	C	350	THR	5.0
1	C	52	TRP	5.0
1	C	221	ALA	5.0
1	C	251	ARG	5.0
1	A	364	ASN	5.0
1	C	364	ASN	5.0
1	B	164	PHE	5.0
1	D	272	PRO	5.0
1	B	318	VAL	5.0
1	C	117	GLU	5.0
1	B	290	ILE	5.0
1	C	97	TRP	5.0
1	B	188	HIS	5.0
1	D	354	LEU	5.0
1	B	278	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	205	VAL	5.0
1	C	65	ASP	5.0
1	C	361	ASP	5.0
1	C	119	TRP	4.9
1	C	156	PRO	4.9
1	C	222	LYS	4.9
1	C	101	VAL	4.9
1	C	177	ASN	4.9
1	B	351	GLN	4.9
1	A	126	GLU	4.9
1	A	9	SER	4.9
1	C	195	SER	4.9
1	D	220	TYR	4.9
1	C	11	GLY	4.9
1	D	209	GLY	4.9
1	D	334	GLY	4.9
1	D	149	ALA	4.9
1	C	121	PRO	4.9
1	B	143	TRP	4.9
1	C	145	TYR	4.9
1	C	281	PHE	4.9
1	D	264	GLY	4.9
1	C	10	THR	4.8
1	D	3	GLY	4.8
1	C	62	PHE	4.8
1	C	173	VAL	4.8
1	C	299	ALA	4.8
1	D	114	ASP	4.8
1	C	370	GLU	4.8
1	C	93	HIS	4.8
1	D	164	PHE	4.8
1	C	206	VAL	4.8
1	D	18	VAL	4.8
1	A	13	ALA	4.8
1	B	89	LEU	4.8
1	A	104	TRP	4.8
1	A	253	ASN	4.7
1	C	282	ASN	4.7
1	A	330	TRP	4.7
1	A	37	GLY	4.7
1	D	282	ASN	4.7
1	D	203	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	4	GLY	4.7
1	A	234	THR	4.7
1	D	302	LEU	4.7
1	C	297	ASN	4.7
1	C	86	LYS	4.7
1	D	25	GLU	4.7
1	C	182	ARG	4.7
1	C	322	MET	4.7
1	A	95	ASP	4.7
1	A	159	ILE	4.7
1	C	241	LYS	4.6
1	C	331	ASP	4.6
1	A	333	ALA	4.6
1	B	279	ALA	4.6
1	A	292	THR	4.6
1	B	328	HIS	4.6
1	C	54	VAL	4.6
1	A	248	LEU	4.6
1	C	178	GLY	4.6
1	C	356	GLY	4.6
1	D	178	GLY	4.6
1	D	222	LYS	4.6
1	A	290	ILE	4.6
1	D	290	ILE	4.6
1	D	285	ASP	4.6
1	A	108	TRP	4.6
1	D	43	ALA	4.5
1	D	281	PHE	4.5
1	C	295	ARG	4.5
1	A	141	TYR	4.5
1	A	276	VAL	4.5
1	C	31	ILE	4.5
1	D	359	ASN	4.5
1	A	346	ALA	4.5
1	A	294	VAL	4.5
1	B	194	VAL	4.5
1	C	346	ALA	4.5
1	D	299	ALA	4.5
1	B	271	GLN	4.4
1	D	184	TRP	4.4
1	A	357	ARG	4.4
1	D	153	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	161	VAL	4.4
1	D	198	LEU	4.4
1	B	124	SER	4.4
1	B	269	MET	4.4
1	A	210	ASP	4.4
1	B	29	ASP	4.4
1	C	189	ALA	4.4
1	C	276	VAL	4.4
1	D	330	TRP	4.4
1	A	220	TYR	4.4
1	A	278	TYR	4.4
1	D	89	LEU	4.4
1	A	215	ILE	4.4
1	C	25	GLU	4.4
1	C	176	GLU	4.4
1	B	239	MET	4.4
1	C	204	LYS	4.4
1	D	237	GLN	4.4
1	B	214	ASN	4.4
1	C	259	SER	4.4
1	C	66	ILE	4.4
1	C	218	PRO	4.4
1	D	298	TYR	4.4
1	D	5	LYS	4.4
1	B	258	THR	4.4
1	D	94	THR	4.4
1	D	259	SER	4.3
1	B	298	TYR	4.3
1	D	296	GLU	4.3
1	C	78	MET	4.3
1	B	209	GLY	4.3
1	A	5	LYS	4.3
1	C	61	LYS	4.3
1	B	115	PRO	4.3
1	D	196	PHE	4.3
1	D	364	ASN	4.3
1	B	97	TRP	4.3
1	C	90	THR	4.3
1	D	42	THR	4.3
1	D	177	ASN	4.3
1	C	74	ILE	4.3
1	C	79	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	31	ILE	4.3
1	C	83	TYR	4.3
1	C	125	ARG	4.3
1	B	260	ALA	4.3
1	C	275	ALA	4.3
1	A	208	GLY	4.3
1	C	300	GLY	4.3
1	D	311	TRP	4.3
1	B	253	ASN	4.3
1	B	280	PHE	4.2
1	C	89	LEU	4.2
1	A	161	VAL	4.2
1	C	87	ILE	4.2
1	D	139	LYS	4.2
1	B	83	TYR	4.2
1	D	132	TYR	4.2
1	C	55	GLU	4.2
1	D	316	ASP	4.2
1	C	311	TRP	4.2
1	C	214	ASN	4.2
1	C	302	LEU	4.2
1	C	9	SER	4.2
1	D	223	GLY	4.2
1	D	331	ASP	4.2
1	D	160	ASN	4.2
1	A	345	ARG	4.2
1	A	272	PRO	4.2
1	B	185	PRO	4.2
1	D	14	PRO	4.2
1	C	286	THR	4.2
1	B	207	PHE	4.2
1	D	87	ILE	4.2
1	C	39	GLY	4.2
1	D	145	TYR	4.2
1	A	153	ASN	4.2
1	C	43	ALA	4.2
1	C	257	HIS	4.1
1	C	59	GLY	4.1
1	A	79	ILE	4.1
1	A	152	ILE	4.1
1	B	284	ASP	4.1
1	C	354	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	40	MET	4.1
1	C	81	ALA	4.1
1	A	145	TYR	4.1
1	D	156	PRO	4.1
1	A	42	THR	4.1
1	A	331	ASP	4.1
1	B	120	GLY	4.1
1	C	56	LEU	4.1
1	D	190	GLY	4.1
1	D	231	CYS	4.1
1	D	83	TYR	4.1
1	C	175	GLN	4.1
1	D	68	SER	4.1
1	D	183	SER	4.1
1	C	304	MET	4.1
1	A	92	LEU	4.1
1	D	84	LEU	4.1
1	D	280	PHE	4.0
1	B	156	PRO	4.0
1	D	158	ASP	4.0
1	A	14	PRO	4.0
1	A	156	PRO	4.0
1	C	163	GLU	4.0
1	D	124	SER	4.0
1	A	300	GLY	4.0
1	D	206	VAL	4.0
1	B	141	TYR	4.0
1	D	225	ASP	4.0
1	C	171	GLU	4.0
1	C	219	GLU	4.0
1	B	359	ASN	4.0
1	D	221	ALA	4.0
1	C	63	ILE	4.0
1	D	33	VAL	4.0
1	D	113	THR	3.9
1	D	19	TYR	3.9
1	D	166	TYR	3.9
1	D	119	TRP	3.9
1	B	362	GLU	3.9
1	B	40	MET	3.9
1	C	58	ASN	3.9
1	D	155	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	262	SER	3.9
1	B	299	ALA	3.9
1	A	280	PHE	3.9
1	D	205	VAL	3.9
1	B	327	ASP	3.9
1	D	255	ASP	3.9
1	A	349	TYR	3.9
1	D	278	TYR	3.9
1	C	103	MET	3.9
1	A	247	GLN	3.9
1	B	197	ALA	3.9
1	C	72	ALA	3.9
1	D	279	ALA	3.9
1	B	264	GLY	3.9
1	D	270	VAL	3.9
1	D	332	VAL	3.9
1	A	263	PHE	3.9
1	C	88	PHE	3.9
1	B	166	TYR	3.9
1	C	287	ARG	3.9
1	C	253	ASN	3.9
1	D	104	TRP	3.9
1	C	28	PRO	3.9
1	A	189	ALA	3.9
1	B	151	THR	3.9
1	B	227	ALA	3.9
1	C	180	THR	3.9
1	A	236	ASP	3.9
1	B	283	ASP	3.9
1	C	179	VAL	3.9
1	B	132	TYR	3.8
1	D	288	TYR	3.8
1	A	286	THR	3.8
1	D	317	ALA	3.8
1	A	34	ILE	3.8
1	B	102	SER	3.8
1	A	84	LEU	3.8
1	A	302	LEU	3.8
1	A	190	GLY	3.8
1	A	226	LEU	3.8
1	D	22	GLY	3.8
1	D	185	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	224	ALA	3.8
1	B	126	GLU	3.8
1	C	268	ASN	3.8
1	C	33	VAL	3.8
1	C	207	PHE	3.8
1	B	315	ARG	3.8
1	C	188	HIS	3.7
1	C	265	GLN	3.7
1	D	115	PRO	3.7
1	B	145	TYR	3.7
1	D	352	TYR	3.7
1	A	275	ALA	3.7
1	C	50	ALA	3.7
1	C	140	ALA	3.7
1	C	205	VAL	3.7
1	C	94	THR	3.7
1	C	15	LYS	3.7
1	B	31	ILE	3.7
1	D	355	ASP	3.7
1	A	362	GLU	3.7
1	A	97	TRP	3.7
1	D	218	PRO	3.7
1	B	125	ARG	3.7
1	C	112	ARG	3.7
1	B	133	ALA	3.7
1	D	349	TYR	3.7
1	C	273	ARG	3.7
1	D	292	THR	3.7
1	B	265	GLN	3.6
1	A	221	ALA	3.6
1	D	224	ALA	3.6
1	A	40	MET	3.6
1	A	222	LYS	3.6
1	A	157	GLY	3.6
1	C	332	VAL	3.6
1	D	310	VAL	3.6
1	A	218	PRO	3.6
1	C	77	LEU	3.6
1	D	165	ASP	3.6
1	D	284	ASP	3.6
1	B	317	ALA	3.6
1	B	349	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	295	ARG	3.6
1	B	37	GLY	3.6
1	B	202	GLY	3.6
1	C	293	GLY	3.6
1	B	247	GLN	3.6
1	D	53	VAL	3.6
1	D	194	VAL	3.6
1	D	219	GLU	3.6
1	B	100	LEU	3.6
1	A	273	ARG	3.6
1	B	184	TRP	3.6
1	B	222	LYS	3.6
1	A	178	GLY	3.6
1	B	69	GLY	3.6
1	B	179	VAL	3.6
1	B	270	VAL	3.6
1	B	314	THR	3.6
1	C	347	SER	3.6
1	B	155	ARG	3.6
1	C	315	ARG	3.6
1	B	77	LEU	3.6
1	D	197	ALA	3.5
1	D	268	ASN	3.5
1	B	52	TRP	3.5
1	C	199	GLU	3.5
1	A	284	ASP	3.5
1	B	191	ASP	3.5
1	B	313	ILE	3.5
1	D	306	THR	3.5
1	A	89	LEU	3.5
1	D	92	LEU	3.5
1	D	261	GLN	3.5
1	C	91	HIS	3.5
1	A	19	TYR	3.5
1	B	19	TYR	3.5
1	B	104	TRP	3.5
1	C	80	PRO	3.5
1	C	130	THR	3.5
1	D	180	THR	3.5
1	A	173	VAL	3.5
1	C	317	ALA	3.5
1	A	269	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	82	ASN	3.5
1	B	172	VAL	3.5
1	B	324	VAL	3.5
1	B	281	PHE	3.5
1	A	48	ALA	3.5
1	B	43	ALA	3.5
1	B	149	ALA	3.5
1	B	257	HIS	3.5
1	C	35	ALA	3.5
1	B	107	GLY	3.5
1	C	131	LYS	3.5
1	D	361	ASP	3.5
1	B	195	SER	3.4
1	B	113	THR	3.4
1	D	141	TYR	3.4
1	A	313	ILE	3.4
1	A	167	ARG	3.4
1	B	310	VAL	3.4
1	C	18	VAL	3.4
1	B	65	ASP	3.4
1	B	165	ASP	3.4
1	B	331	ASP	3.4
1	B	355	ASP	3.4
1	C	227	ALA	3.4
1	D	227	ALA	3.4
1	B	272	PRO	3.4
1	A	298	TYR	3.4
1	C	269	MET	3.4
1	A	266	ILE	3.4
1	B	91	HIS	3.4
1	B	93	HIS	3.4
1	C	313	ILE	3.4
1	D	143	TRP	3.4
1	D	161	VAL	3.4
1	D	265	GLN	3.4
1	B	319	THR	3.4
1	C	32	ARG	3.4
1	A	83	TYR	3.4
1	D	17	TYR	3.4
1	C	362	GLU	3.4
1	A	285	ASP	3.4
1	A	316	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	191	ASP	3.4
1	A	175	GLN	3.4
1	D	157	GLY	3.4
1	B	276	VAL	3.4
1	C	134	VAL	3.4
1	A	72	ALA	3.4
1	A	168	ALA	3.4
1	C	51	ALA	3.4
1	B	177	ASN	3.4
1	B	196	PHE	3.4
1	A	233	MET	3.4
1	B	180	THR	3.4
1	B	292	THR	3.4
1	C	128	MET	3.4
1	C	258	THR	3.4
1	C	165	ASP	3.3
1	D	191	ASP	3.3
1	C	57	GLY	3.3
1	C	148	ARG	3.3
1	A	25	GLU	3.3
1	C	326	PRO	3.3
1	C	17	TYR	3.3
1	D	34	ILE	3.3
1	C	333	ALA	3.3
1	D	105	ALA	3.3
1	B	25	GLU	3.3
1	D	286	THR	3.3
1	C	301	PRO	3.3
1	D	200	TRP	3.3
1	B	210	ASP	3.3
1	C	355	ASP	3.3
1	A	347	SER	3.3
1	C	124	SER	3.3
1	C	288	TYR	3.3
1	B	49	ALA	3.3
1	B	81	ALA	3.3
1	B	329	ALA	3.3
1	C	279	ALA	3.3
1	C	305	ALA	3.3
1	D	275	ALA	3.3
1	B	158	ASP	3.3
1	C	213	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	295	ARG	3.3
1	B	119	TRP	3.3
1	C	330	TRP	3.3
1	C	170	ASN	3.3
1	C	190	GLY	3.3
1	D	15	LYS	3.2
1	B	274	HIS	3.2
1	D	91	HIS	3.2
1	D	159	ILE	3.2
1	B	161	VAL	3.2
1	B	236	ASP	3.2
1	D	179	VAL	3.2
1	A	115	PRO	3.2
1	C	120	GLY	3.2
1	C	208	GLY	3.2
1	A	71	MET	3.2
1	A	200	TRP	3.2
1	B	186	CYS	3.2
1	C	162	HIS	3.2
1	A	187	ILE	3.2
1	B	114	ASP	3.2
1	B	287	ARG	3.2
1	C	20	TYR	3.2
1	C	158	ASP	3.2
1	C	283	ASP	3.2
1	D	236	ASP	3.2
1	D	321	ARG	3.2
1	A	50	ALA	3.2
1	B	277	ALA	3.2
1	A	100	LEU	3.2
1	B	163	GLU	3.2
1	D	23	SER	3.2
1	D	103	MET	3.2
1	B	231	CYS	3.2
1	B	95	ASP	3.2
1	B	350	THR	3.2
1	D	38	THR	3.2
1	D	174	TYR	3.2
1	C	21	PRO	3.2
1	B	54	VAL	3.2
1	C	71	MET	3.2
1	B	27	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	183	SER	3.2
1	D	120	GLY	3.2
1	B	88	PHE	3.2
1	A	144	ASP	3.2
1	B	286	THR	3.1
1	A	20	TYR	3.1
1	B	291	TYR	3.1
1	A	270	VAL	3.1
1	A	303	SER	3.1
1	A	318	VAL	3.1
1	B	33	VAL	3.1
1	D	118	VAL	3.1
1	A	237	GLN	3.1
1	C	261	GLN	3.1
1	B	147	THR	3.1
1	D	235	SER	3.1
1	A	155	ARG	3.1
1	D	39	GLY	3.1
1	D	106	GLY	3.1
1	B	101	VAL	3.1
1	B	138	LEU	3.1
1	B	131	LYS	3.1
1	B	297	ASN	3.1
1	D	170	ASN	3.1
1	C	314	THR	3.1
1	A	212	ALA	3.1
1	A	260	ALA	3.1
1	A	325	SER	3.1
1	B	50	ALA	3.1
1	D	193	PRO	3.1
1	C	223	GLY	3.1
1	A	179	VAL	3.1
1	B	206	VAL	3.1
1	B	268	ASN	3.1
1	C	267	MET	3.1
1	A	258	THR	3.1
1	A	314	THR	3.1
1	D	303	SER	3.1
1	A	301	PRO	3.1
1	B	46	ALA	3.1
1	B	159	ILE	3.0
1	D	353	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	103	MET	3.0
1	D	238	MET	3.0
1	C	201	ASN	3.0
1	A	281	PHE	3.0
1	A	289	ASP	3.0
1	C	244	GLN	3.0
1	C	146	MET	3.0
1	B	296	GLU	3.0
1	C	76	SER	3.0
1	C	144	ASP	3.0
1	C	272	PRO	3.0
1	A	224	ALA	3.0
1	C	34	ILE	3.0
1	D	64	VAL	3.0
1	B	190	GLY	3.0
1	D	4	GLY	3.0
1	A	142	ASN	3.0
1	B	176	GLU	3.0
1	A	228	ILE	3.0
1	A	257	HIS	2.9
1	B	96	HIS	2.9
1	C	84	LEU	2.9
1	B	237	GLN	2.9
1	D	356	GLY	2.9
1	D	326	PRO	2.9
1	A	296	GLU	2.9
1	D	97	TRP	2.9
1	A	277	ALA	2.9
1	A	31	ILE	2.9
1	B	112	ARG	2.9
1	D	125	ARG	2.9
1	C	64	VAL	2.9
1	A	203	TYR	2.9
1	A	149	ALA	2.9
1	A	91	HIS	2.9
1	A	93	HIS	2.9
1	A	311	TRP	2.9
1	D	175	GLN	2.9
1	D	26	LEU	2.9
1	A	304	MET	2.9
1	B	238	MET	2.9
1	A	123	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	57	GLY	2.9
1	C	141	TYR	2.9
1	A	21	PRO	2.9
1	A	88	PHE	2.9
1	B	168	ALA	2.9
1	C	138	LEU	2.9
1	A	293	GLY	2.9
1	C	22	GLY	2.9
1	A	306	THR	2.8
1	C	312	ASN	2.8
1	A	174	TYR	2.8
1	D	20	TYR	2.8
1	A	125	ARG	2.8
1	A	287	ARG	2.8
1	B	15	LYS	2.8
1	A	46	ALA	2.8
1	D	72	ALA	2.8
1	D	181	PHE	2.8
1	C	127	ASP	2.8
1	B	303	SER	2.8
1	D	269	MET	2.8
1	D	79	ILE	2.8
1	B	300	GLY	2.8
1	D	27	GLY	2.8
1	D	271	GLN	2.8
1	D	274	HIS	2.8
1	B	139	LYS	2.8
1	A	166	TYR	2.8
1	A	255	ASP	2.8
1	D	88	PHE	2.8
1	D	36	CYS	2.8
1	D	82	ASN	2.8
1	B	106	GLY	2.8
1	A	188	HIS	2.8
1	B	117	GLU	2.8
1	C	135	GLU	2.8
1	C	230	GLU	2.8
1	D	304	MET	2.8
1	C	23	SER	2.8
1	B	142	ASN	2.8
1	C	157	GLY	2.8
1	C	328	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLU	2.8
1	D	230	GLU	2.8
1	B	63	ILE	2.8
1	B	87	ILE	2.8
1	B	311	TRP	2.8
1	A	53	VAL	2.8
1	B	201	ASN	2.7
1	B	346	ALA	2.7
1	D	49	ALA	2.7
1	C	36	CYS	2.7
1	A	39	GLY	2.7
1	C	123	GLY	2.7
1	D	208	GLY	2.7
1	A	169	LEU	2.7
1	B	226	LEU	2.7
1	C	60	ASP	2.7
1	D	52	TRP	2.7
1	C	19	TYR	2.7
1	D	277	ALA	2.7
1	D	293	GLY	2.7
1	D	301	PRO	2.7
1	C	82	ASN	2.7
1	B	48	ALA	2.7
1	A	334	GLY	2.7
1	D	78	MET	2.7
1	B	262	SER	2.7
1	B	219	GLU	2.7
1	A	64	VAL	2.7
1	B	134	VAL	2.7
1	C	27	GLY	2.6
1	B	146	MET	2.6
1	C	289	ASP	2.6
1	C	16	ARG	2.6
1	B	26	LEU	2.6
1	B	84	LEU	2.6
1	C	192	GLY	2.6
1	D	107	GLY	2.6
1	D	267	MET	2.6
1	D	300	GLY	2.6
1	B	305	ALA	2.6
1	C	306	THR	2.6
1	A	186	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	204	LYS	2.6
1	B	347	SER	2.6
1	D	312	ASN	2.6
1	B	16	ARG	2.6
1	D	29	ASP	2.6
1	A	101	VAL	2.6
1	A	134	VAL	2.6
1	A	219	GLU	2.6
1	D	323	ALA	2.6
1	A	177	ASN	2.6
1	A	214	ASN	2.6
1	A	121	PRO	2.6
1	C	45	ARG	2.6
1	B	175	GLN	2.6
1	A	35	ALA	2.6
1	A	73	ASN	2.6
1	B	306	THR	2.6
1	C	85	THR	2.6
1	C	96	HIS	2.5
1	B	174	TYR	2.5
1	C	132	TYR	2.5
1	A	196	PHE	2.5
1	A	138	LEU	2.5
1	B	66	ILE	2.5
1	D	67	GLY	2.5
1	D	324	VAL	2.5
1	B	182	ARG	2.5
1	C	186	CYS	2.5
1	D	201	ASN	2.5
1	D	93	HIS	2.5
1	A	265	GLN	2.5
1	A	324	VAL	2.5
1	B	199	GLU	2.5
1	D	117	GLU	2.5
1	D	65	ASP	2.5
1	C	139	LYS	2.5
1	B	198	LEU	2.5
1	D	96	HIS	2.5
1	A	267	MET	2.5
1	D	350	THR	2.5
1	A	231	CYS	2.4
1	B	273	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	123	GLY	2.4
1	A	162	HIS	2.4
1	B	24	GLU	2.4
1	B	229	HIS	2.4
1	C	75	GLN	2.4
1	C	303	SER	2.4
1	D	347	SER	2.4
1	B	34	ILE	2.4
1	B	60	ASP	2.4
1	D	63	ILE	2.4
1	A	305	ALA	2.4
1	B	53	VAL	2.4
1	B	320	GLU	2.4
1	C	98	GLY	2.4
1	D	322	MET	2.4
1	B	259	SER	2.4
1	B	181	PHE	2.4
1	B	94	THR	2.4
1	D	74	ILE	2.4
1	D	362	GLU	2.4
1	A	172	VAL	2.4
1	D	276	VAL	2.4
1	C	327	ASP	2.3
1	C	44	ARG	2.3
1	A	10	THR	2.3
1	D	85	THR	2.3
1	C	351	GLN	2.3
1	A	323	ALA	2.3
1	B	51	ALA	2.3
1	B	323	ALA	2.3
1	D	50	ALA	2.3
1	A	80	PRO	2.3
1	A	322	MET	2.3
1	D	146	MET	2.3
1	D	37	GLY	2.3
1	D	102	SER	2.3
1	D	357	ARG	2.3
1	D	348	GLU	2.3
1	D	138	LEU	2.3
1	B	136	HIS	2.3
1	A	43	ALA	2.3
1	B	140	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	37	GLY	2.3
1	C	316	ASP	2.3
1	B	171	GLU	2.3
1	B	56	LEU	2.3
1	B	302	LEU	2.3
1	A	201	ASN	2.3
1	C	137	MET	2.3
1	A	140	ALA	2.3
1	A	202	GLY	2.3
1	A	264	GLY	2.3
1	C	102	SER	2.3
1	C	325	SER	2.3
1	D	144	ASP	2.3
1	D	171	GLU	2.3
1	D	327	ASP	2.3
1	C	310	VAL	2.3
1	B	170	ASN	2.3
1	C	100	LEU	2.3
1	D	148	ARG	2.2
1	D	62	PHE	2.2
1	B	289	ASP	2.2
1	D	95	ASP	2.2
1	A	205	VAL	2.2
1	B	267	MET	2.2
1	C	296	GLU	2.2
1	A	27	GLY	2.2
1	B	59	GLY	2.2
1	B	144	ASP	2.2
1	C	70	SER	2.2
1	D	28	PRO	2.2
1	D	283	ASP	2.2
1	D	289	ASP	2.2
1	A	229	HIS	2.2
1	D	229	HIS	2.2
1	B	71	MET	2.2
1	C	324	VAL	2.2
1	D	163	GLU	2.2
1	A	49	ALA	2.2
1	C	309	MET	2.2
1	A	47	GLN	2.2
1	C	271	GLN	2.2
1	B	42	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	2.2
1	B	122	SER	2.2
1	A	223	GLY	2.2
1	D	59	GLY	2.2
1	A	282	ASN	2.1
1	A	119	TRP	2.1
1	B	316	ASP	2.1
1	A	96	HIS	2.1
1	B	72	ALA	2.1
1	C	142	ASN	2.1
1	D	58	ASN	2.1
1	D	81	ALA	2.1
1	A	124	SER	2.1
1	D	32	ARG	2.1
1	D	24	GLU	2.1
1	B	78	MET	2.1
1	B	326	PRO	2.1
1	A	268	ASN	2.1
1	A	227	ALA	2.1
1	D	46	ALA	2.1
1	B	285	ASP	2.1
1	A	44	ARG	2.1
1	A	76	SER	2.1
1	D	45	ARG	2.1
1	B	123	GLY	2.1
1	C	129	GLY	2.1
1	A	78	MET	2.1
1	B	137	MET	2.1
1	D	328	HIS	2.1
1	D	21	PRO	2.1
1	A	198	LEU	2.1
1	B	148	ARG	2.1
1	A	164	PHE	2.0
1	C	126	GLU	2.0
1	A	274	HIS	2.0
1	D	192	GLY	2.0
1	A	206	VAL	2.0
1	A	81	ALA	2.0
1	C	49	ALA	2.0
1	B	127	ASP	2.0
1	A	129	GLY	2.0
1	B	85	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	178	GLY	2.0
1	C	47	GLN	2.0
1	A	18	VAL	2.0
1	A	148	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

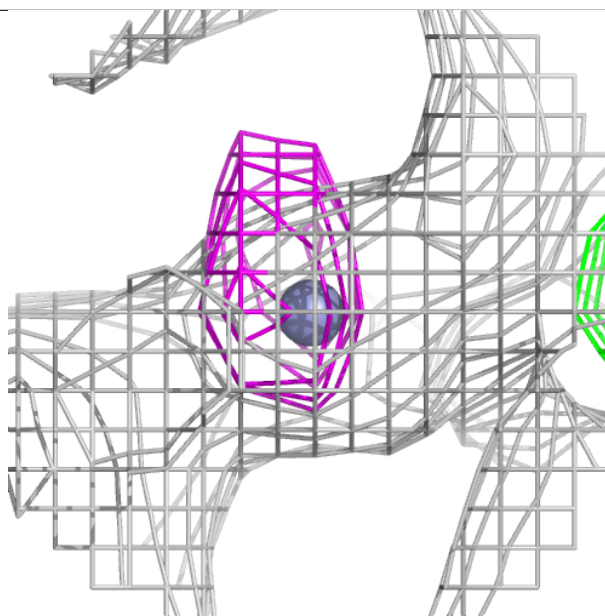
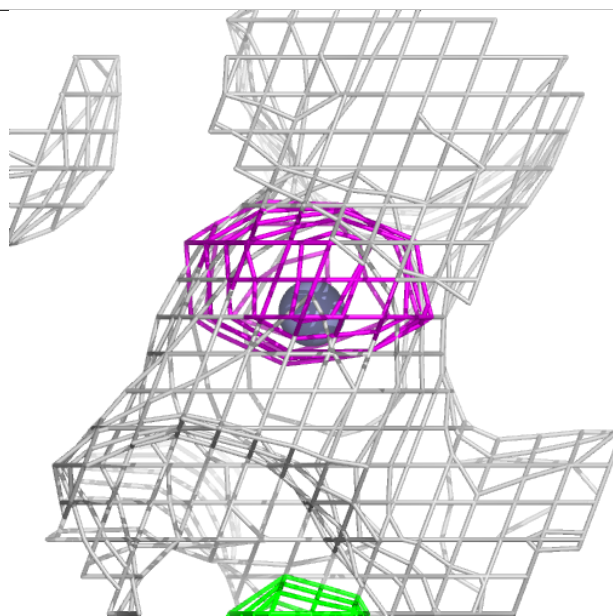
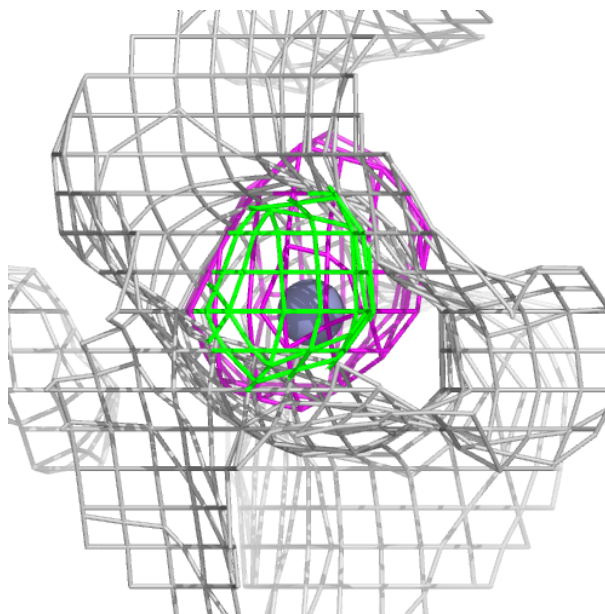
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	401	1/1	0.84	0.35	33,33,33,33	0
2	ZN	C	401	1/1	0.85	0.25	45,45,45,45	0
2	ZN	D	401	1/1	0.89	0.08	43,43,43,43	0
2	ZN	A	401	1/1	0.97	0.40	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

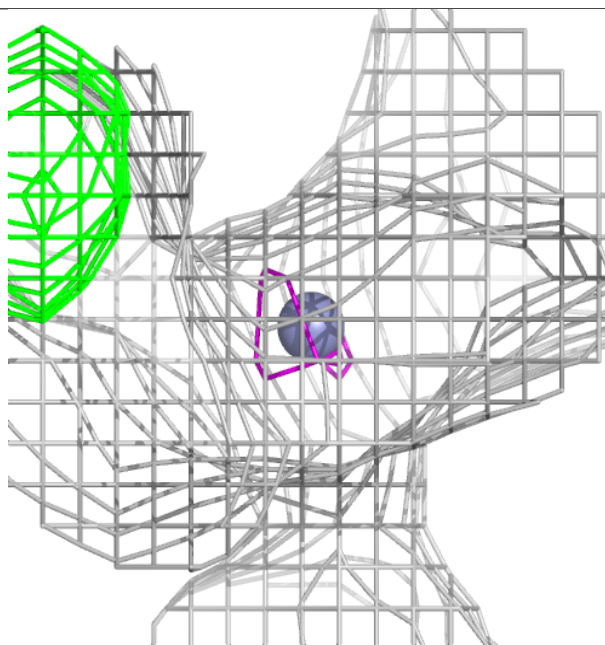
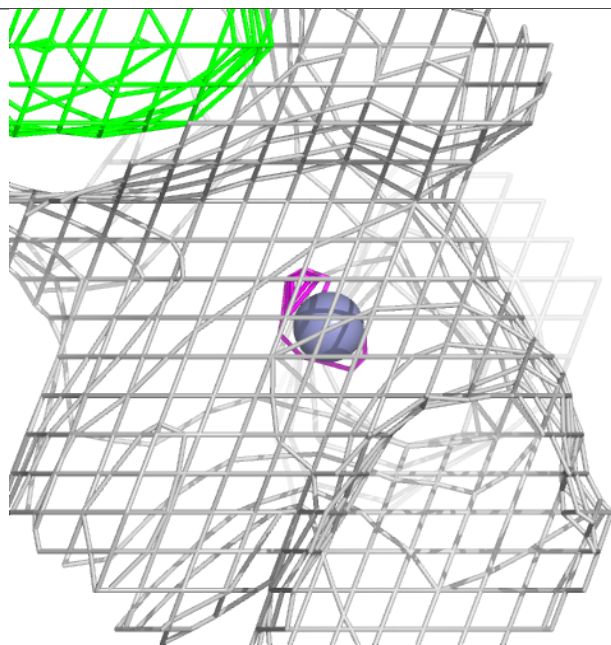
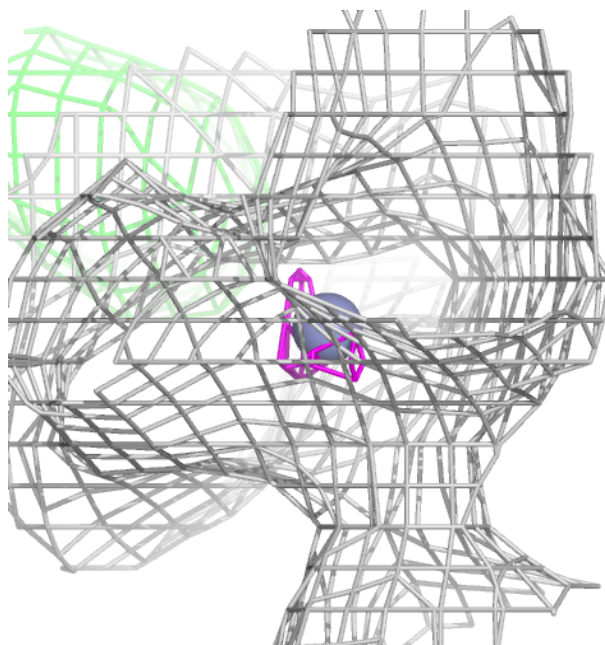
Electron density around ZN B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



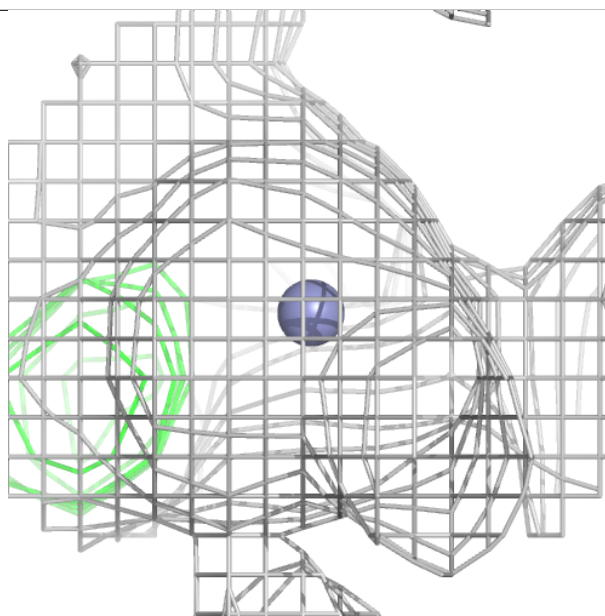
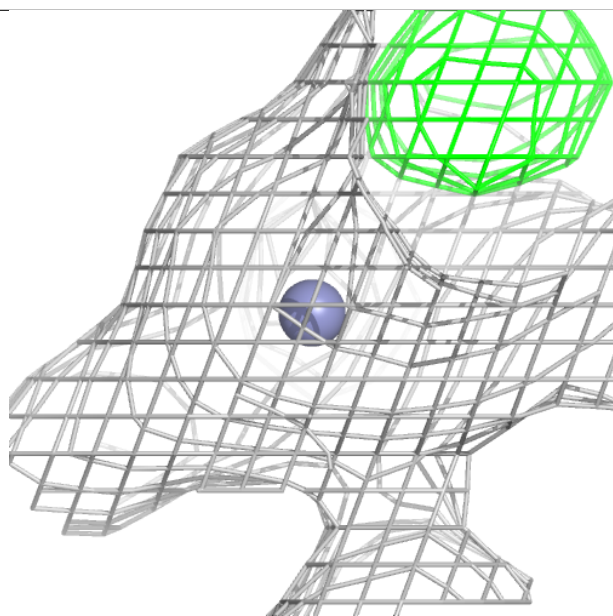
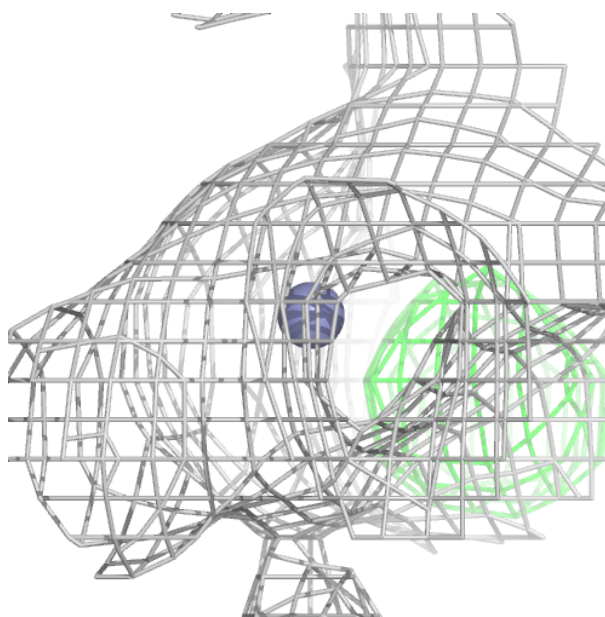
Electron density around ZN C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



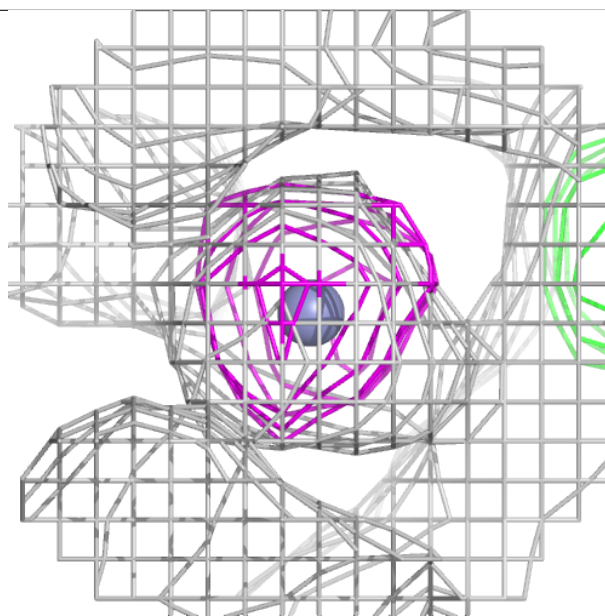
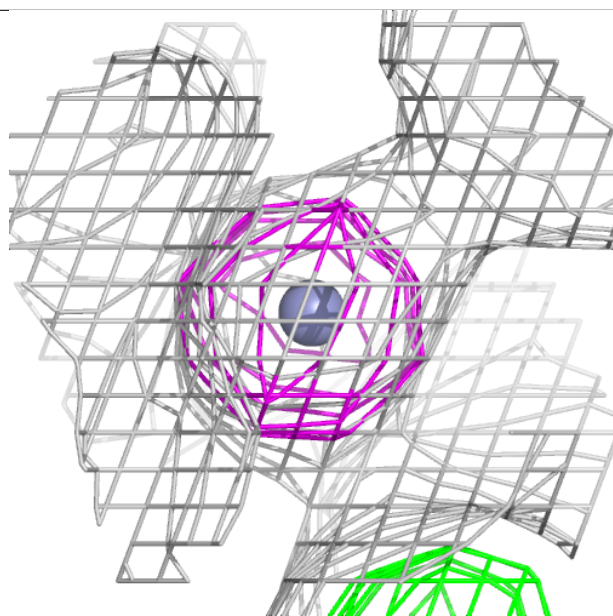
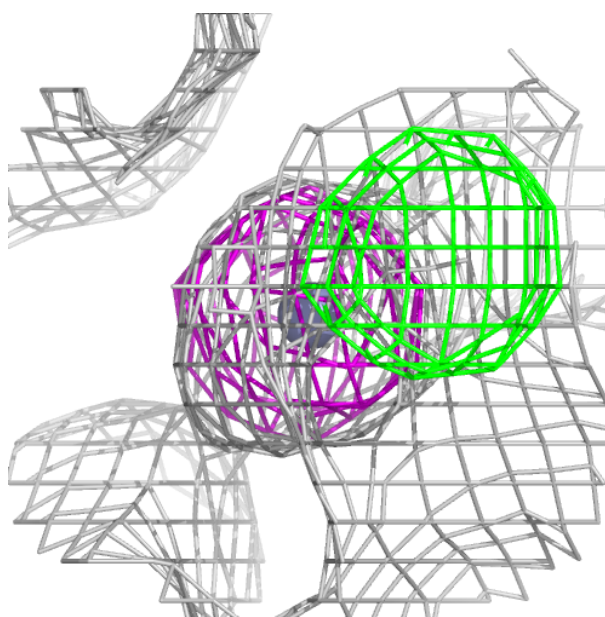
Electron density around ZN D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.